Proceedings of CTTC - 2024

Proceedings of

DAE-BRNS Symposium on
^{64}Current ^{3}Trends in ^{232}Theoretical ^{13}Chemistry
(CTTC-2024)

September 26-28, 2024

Chemistry Division
Bhabha Atomic Research Centre, Mumbai – 400085, INDIA

Sponsored by

BRNS

In Association with

Society for Materials Chemistry

CTTC – 2024

Proceedings of
DAE-BRNS Symposium on
Current Trends in Theoretical Chemistry

Bhabha Atomic Research Centre Mumbai, India
September 26 – 28, 2024

Organised by

Chemistry Division
Bhabha Atomic Research Centre
Trombay, Mumbai-400 085, India
In association with
Society for Materials Chemistry, India

Sponsored by

Board of Research in Nuclear Sciences (BRNS),
Department of Atomic Energy, GOI

सीटीटीसी – 2024

सैद्धांतिक रसायन शास्त्र में समसामयिक विचारधाराओं पर पऊवि बीआरएनएस संगोष्ठी की कार्यवाही

भाभा परमाणु अनुसंधान केंद्र , मुबंई – 400085, भारत
सितंबर 26 – 28, 2024

आयोजक
रसायनिकी प्रभाग , भाभा परमाणु अनुसंधान केंद्र
पऊवि, मुबंई – 400085, भारत
सह प्रायोजक
पदार्थ रसायनिकी हेतु संस्था, मुबंई, भारत

प्रायोजक
बीआरएनएस, पऊवि, भारत

Proceedings of

DAE-BRNS Symposium on

Current Trends in Theoretical Chemistry (CTTC- 2024)

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Scientific Programme ⬇

CTTC-2024 Proceedings ⬇

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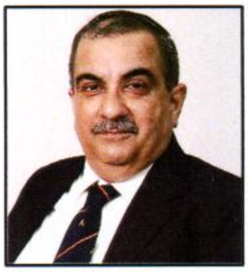

MESSAGE

I am happy to learn that Chemistry Division, Bhabha Atomic Research Centre, is organizing the DAE-BRNS symposium on "Current Trends in Theoretical Chemistry (CTTC-2024)" during September 26-28, 2024 at DAE Convention Centre, Anushaktinagar, Mumbai.

Chemistry has been an important component of India's Nuclear Energy Programme since its inception. Theoretical Chemistry, which deals with quantum nature of electrons to elucidate properties of materials and their underlying behavior, plays a pivotal role in both front and back end of the nuclear fuel cycles of the Indian nuclear energy programme. Predicting the effect of fission products on fuel properties, computational design of ligands for effective extraction of radioactive ions from aqueous solution of spent fuels, understanding radiation damages in nuclear structural materials, predicting migration behavior of radioactive ions in underground soil clays are some of the important areas of research carried out in BARC. Theoretical chemistry has immense contributions in many recent research areas, like development of materials for generation and storage of hydrogen, catalysts for water splitting, understanding protein-drug interactions, etc. Recent developments in artificial intelligence and data mining have strengthen theoretical and computational chemistry with better predictability, leading to accelerated discovery of new molecules and materials. With the advent of high performance supercomputing machines, theoretical and computational chemistry has become an inevitable part of chemical research with strong interface with other branches of science and engineering.

I congratulate Chemistry Group for planning this Symposium, which will provide a forum for close interactions of BARC scientists from various disciplines with the leading theoretical chemists of the country. I am confident that the Symposium will highlight current trends and set the future directions of theoretical and computational chemistry, benefiting both young and established researchers. It will also provide an opportunity for interdisciplinary collaborative research among the leading research groups in the country.

I wish all the success to CTTC-2024.

Vivek Bhasin

23.09.2024

(Vivek Bhasin)

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Dean

प्रो. ए. के. त्यागी
(FNASc, FASc, FNAE, FNA, FTWAS)
डीन

Foreword

It gives me immense pleasure to write FOREWORD for The DAE-BRNS symposium on the 'Current Trends in Theoretical Chemistry (CTTC-2024)' which is being organised by the Chemistry Division, Bhabha Atomic Research Centre, Mumbai in association with the Society for Materials Chemistry during 26-28 September, 2024 at DAE Convention Centre, Anushaktinagar, Mumbai.

Chemistry, in general, deals with the study of composition, structure and properties of elements, molecules and materials and the chemical reactions. Chemistry is intimately associated with major areas the modern society like food, health, energy and environment. Over the years, theoretical chemistry has emerged as an important and integral part of Chemistry. In recent years, the development of fundamental concepts as well as mathematical foundations within the domain of theoretical chemistry has increased tremendously without any ambiguity, especially with the advancement of state-of-the-art computational techniques. The primary goal of theoretical chemistry is to provide an in-depth understanding and rationalization of the observed chemical phenomena as well as to predict new phenomena by developing concepts or performing computations with the help of the available theoretical, modeling, or simulation techniques. Formulation of new and more powerful theoretical tools, modeling strategies and simulation techniques thus forms an ongoing and integral part of research activities in theoretical chemistry. Proposing new experiments, guided by theoretical insights, also constitute a valuable component of research in theoretical chemistry. With the advent of artificial intelligence and machine learning, along with high performance computing facilities, predictability of theoretical chemistry has increased many folds. Scientists can now screen large database of materials to identify top performing candidates for various applications like gas separation & storage, computational design of catalytic and photovoltaic materials etc. thereby significantly reducing the experimental efforts. The objective of CTTC-2024 is to provide a fertile ground for intense discussion on the thriving newer areas in theoretical chemistry and thereby setting up the course for future directions and shedding light into potentially more powerful applications of theoretical chemistry in interdisciplinary areas. The symposium covers a wide variety of topics that include recent advances in the Theoretical Formalisms and Simulation Methodologies, Machine Learning and Artificial Intelligence in Chemistry, Modeling, Theory, and Simulation in Nuclear Fuel and Waste Management Research, Theoretical and Computational Chemistry in Understanding Radiation Damages in Nuclear Materials, Theoretical Design of Molecules and Materials Pertaining to Energy Research, Modeling, Theory, and Simulation in Soft Condensed Matter, Electronic Structure and Spectroscopy of Atoms, Molecules, Clusters, Nanomaterials, and Solids, and Materials under Extreme Conditions, Experiment Driven Theoretical Investigations, Modeling, Theory and Simulation for the Exploration of Biological Phenomena and Drug Design. The present symposium will provide a scientifically motivating environment for intense discussions and exchange of innovative ideas among the delegates and will lead to fruitful interdisciplinary collaborative research activities in the country.

The valuable inputs and advices from all the members of the National Advisory Committee are sincerely acknowledged. All the participants are thanked for their interest and enthusiasm which is highly essential for making this symposium a grand success. We welcome all the delegates and hope this platform will be scientifically enriching experience.

(A. K. Tyagi)
Chairman, CTTC-2024

R & D Activities of Chemistry Division

Chemical sciences, in general, have played an important role in India's indigenous nuclear energy programme. This has led to the initiation of chemistry activities in the Atomic Energy Establishment, Trombay way back in 1949. Currently, Chemistry Group encompasses five divisions; among these three Divisions, namely, Analytical Chemistry Division, Chemistry Division, and Radiation & Photochemistry Division, are located at Trombay, Mumbai and other two Divisions, National Centre for Compositional Characterisation of Materials and Water and Steam Chemistry Division are located at Hyderabad and BARC-Facilities, IGCAR, Kalpakkam, respectively. . Chemistry Division is the oldest Division of Chemistry Group. Its mandate has been to undertake both advanced basic and applied research in thrust areas of DAE's vision programme. The major scientific activities of the Division are: Research & Development of materials for nuclear energy, hydrogen energy, catalysis, healthcare, bio-sensors, high-purity materials, functional materials, toxic gas sensors & detectors, development of theoretical methods and applications of computational chemistry in DAE related activities.

R & D in the area of nuclear materials primarily focuses on evaluation of thermo-physical and chemical properties of materials relevant to nuclear fuel cycles. Some of the activities in this area include research in sacrificial core catcher materials, materials for immobilization of actinides or lanthanides, as well as radiation stable materials. Useful thermodynamic and thermo-physical properties generated for molten salts have a direct relevance to the development of Molten Salt Breeder Reactors (MSBR). The Division also has made important contributions in the area of hydrogen generation and storage materials, component materials for intermediate temperature solid oxide fuel cells and catalysts for mitigation of hydrogen in nuclear power plants under severe accident conditions, etc. Under the affordable healthcare research program, efforts are being made for the development of nano drug delivery systems for anticancer drugs, nutraceuticals, etc. With the objective of providing an impetus to the development of indigenous radiation detectors, a program has been undertaken to develop organic compounds-based scintillation detectors and their implementation in radiation monitoring systems.

Theoretical Chemistry Section (TCS) of Chemistry Division, BARC has advanced cutting-edge research in theoretical and computational modelling of materials at various length and time scales over the years. The primary goal of TCS has been to provide an in-depth understanding and rationalization of the observed chemical phenomena and more importantly, to predict new materials with tailor-made properties through the development of new concepts and the use of available computational tools. TCS is also involved in multi-scale modelling of molecules, clusters and materials that cover microscopic, mesoscopic and macroscopic length scales dealing with the electronic structure, atomistic theory and simulation, and continuum descriptions, respectively. Some of the notable contributions include developing new methods based on density functional theory and conceptual density functional theory, statistical mechanics based models to calculate the transport properties of fluids, electron transfer reactions in condensed phases, new methodologies for molecular dynamics (MD) and Monte Carlo (MC) simulation techniques, non-equilibrium solvation dynamics, *ab initio* quantum chemical methodologies for computing the autoionizing electronic resonance states, implementation of a new property module to the recently released version of widely used DIRAC10 program package, modelling materials for hydrogen generation and storage, electronic structure and thermo-physical properties for advanced nuclear fuel materials, structural integrity of DNA against the attack by very-low energy electron, binding and un-binding mechanism of uranyl ion from the ion binding-site of human serum albumin, photo-catalytic and thermo-luminescent materials, porous materials for gas separation and storage, etc. Recent advancements in the state-of-the-art techniques, such as machine learning and high-throughput screening techniques have also been employed for designing materials for energy, environment and healthcare.

The various research projects that have been undertaken have produced a number of cutting-edge innovations as well as publications in peer-reviewed journals, scientific bulletins, BARC News Letter, etc. A few indigenous instruments were also developed for in-house R&D work. Chemistry Division is credited with the transfer of several technologies toward commercialization. The division is well-equipped with major instruments like XPS, powder XRD, High Temperature XRD, Rotating Anode XRD, Single Crystal XRD, Small Angle X-ray Scattering, multinuclear NMR, TG-DTA, SEM, AFM, etc. Chemistry Division is also actively participating in collaborative projects with other research groups in BARC/ DAE, Universities (both in India and abroad)/ National Institutes through BRNS schemes, DST, international collaborations, etc. Many colleagues have received important honors from scientific organizations, and fellowships from science academies. We take this opportunity to compliment all the colleagues for their sustained excellence in diverse areas relevant to the departmental programmes, and look forward to their making greater strides in coming years.

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DAE-BRNS Symposium on Current Trends in Theoretical Chemistry

सैद्धांतिक रसायन शास्त्र में समसामयिक विचारधाराओं पर पऊवि बीआरएनएस संगोष्ठी

Bhabha Atomic Research Centre, Mumbai, India

September 26 – 28, 2024

भाभा परमाणु अनुसंधान केंद्र, मुंबई – 400085, भारत

सितंबर 26 – 28, 2024

Day -1, 26th September 2024 (Thursday)

Time		
9:30 – 10:30	***Inaugural Function & Keynote address by the Chief Guest***	
10:30 – 11:00	***High Tea***	
11:00 – 12:20	***Plenary Session 1*** **Session Chair: Prof. A. K. Tyagi**	
11:00 – 11:40	**PL-1: Prof. Sourav Pal, Ashoka University** *Accurate methods for shape resonance and decay processes in molecules*	
11:40 – 12:20	**PL-2: Prof. Rajeev Ahuja, IIT Ropar** *Computational Materials Science and Its Applications in The Area of Materials for Energy*	
12:20 – 13:20	***Session 1*** **Session Chair: Prof. Awadhesh Kumar**	
12:20 – 12:50	Perspective Talk - 1	**Prof. Prabal K. Maiti, IISc, Bangaluru** *2-TIPS and ordering in various active matter systems*
12:50 – 13:20	Perspective Talk - 2	**Prof. Sanjoy Bandyopadhyay, IIT Kharagpur** *Interfacial Properties of Biomolecules in Aqueous Ionic Liquid Solution*
13:20 – 14:00	***Lunch Break***	
14:00 – 15:45	***Session 2*** **Session Chair: Prof. A. C. Bhasikuttan**	
14:00 – 14:30	Perspective Talk - 3	**Prof. Ashok Arya, BARC, Mumbai** *Efficient screening of single phase forming low-activation high entropy alloys*
14:30 – 15:00	Perspective Talk – 4	**Prof. Suman Chakrabarty, S N Bose National Centre for Basic Sciences, Kolkata** *Exploration of Free Energy Landscape of Complex Molecular Systems: Dynamics to Thermodynamics and Back*
15:00 – 15:30	Perspective Talk - 5	**Prof. Dilip K. Maity, BARC, Mumbai** *Hydration of metal ions and molecules*
15:30 – 15:45	LT-1	**Prof. Anoop Ayyappan, Digital University Kerala** *Exploring Boron Group Nanoclusters for Catalytic Activity*
15:45 – 16:00	Technical Talk-1	**Netweb Technologies**
16:00 – 16:15	***Tea Break***	
16:15 – 18:15	***Session 3*** **Session Chair: Prof. S. R. Gadre & Prof. V. Subramanian**	
16:15 – 16:45	Perspective Talk - 6	**Prof. Gour P. Das, TCG CREST, Kolkata** *Quo Vadis DFT:a Perspective*
16:45 – 17:15	Perspective Talk - 7	**Prof. Pratim K. Chattaraj, BIT Mesra** *Global Optimization of Atomic Clusters: A Soft Computing Perspective*
17: 15 –17:45	Perspective Talk – 8	**Prof. Alok K. Samanta, Former BARC, Mumbai** *A new approach to a Generalized Smoluchowski Equation*
17: 45 –18:15	Perspective Talk - 9	**Prof. Chandra N. Patra, BARC, Mumbai** *Large Molecules in Solution: Multiscale Modeling and Simulation*
18:15 – 19:00	**Session Chair: Prof. J. P. Mittal**	
18:15 – 19:00	Evening Lecture	**Prof. Swapan K. Ghosh, UM-DAE CEBS, Mumbai**
19:30 Onwards		**Banquet Dinner**

Day -2, 27th September 2024 (Friday)

Time				
9:30 – 10:15	***Plenary Session 2*** **Session Chair: Prof. S. K. Ghosh**			
9:30 – 10:15	**PL-3**	**Prof. Biman Bagchi, IISc, Bangaluru** *Memory Effects and Quantum Coherence in Excitation Energy Transfer in Photosynthetic Reaction Systems*		
10:15 – 11:15	**Session 4** **Session Chair: Prof. Pratim K Chattaraj**			
10:15 – 10:45	**Perspective Talk – 10**	**Prof. Satrajit Adhikari, IACS Kolkata** *The effect of surface temperature on molecule-surface scattering processes*		
10:45 – 11:15	**Perspective Talk – 11**	**Prof. Nisanth N. Nair, IIT Kanpur** *Exploring Rugged Energy Landscapes of Enzymatic Reactions*		
11:15 – 11:30	***Tea Break***			
11:30 – 13:10	***Session 5*** **Session Chair: Prof. Y. K. Bhardwaj & Prof. C. Majumder**			
11:30 – 12:00	**Perspective Talk – 12**	**Prof. Amalendu Chandra, IIT Kanpur** *Terahertz Spectroscopy of Aqueous Systems using Polarizable Models*		
12:00 – 12:30	**Perspective Talk – 13**	**Prof. Biman Jana, IACS Kolkata** *Optimizing Collective Variable for Linear Hydrophobic Polymer Collapse and Protein Folding Transitions: Crucial Role of Hydration*		
12:30 – 12:50	**ST-1**	**Prof. Arup K. Pathak, BARC, Mumbai** *Uranyl Ion Binding to Human Serum Albumin: Influence of Fatty Acid*		
12:50 – 13:10	**ST-2**	**Prof. Mahesh Sundararajan, BARC, Mumbai** *Theory Driven Experiments for Small Molecule Activation*		
13:10 – 14:00	**Lunch Break**			
14:00 – 15:30	***Poster Session & Tea*** **(Categories: A to F)** **Session Chairs: Prof. V. Sudarsan & Prof. S. Sahoo** **(Members: Profs. R. Acharya, Y. Sajeev, B. Modak, S. Nath, S. N. Achary, J. Jose, R. Mahesh, J. Mohanty, M. C. Rath, C. A. Betty)**			
15:30 – 17:15	***Session 6*** **Session Chair: Prof. S. M. Yusuf**			
15:30 – 16:00	**Perspective Talk – 14**	**Prof. Ranjit Biswas, S N Bose National Centre for Basic Sciences, Kolkata** *Liquid Phase of Deep Eutectics: Enthalpy versus Entropy*		
16:00 – 16:30	**Perspective Talk – 15**	**Prof. Sk. Musharaf Ali, BARC, Mumbai** *Dehydration Induced Selective Ion Trapping by Topology Constrained Atomically Thin Graphene-Crown Membranes*		
16:30 – 17:00	**Perspective Talk – 16**	**Prof. B. V. R. Tata, GITAM University, Vizag** *Unusual Dynamics, Phase Behavior and Yielding of Dense Stimuli Responsive Microgel Glasses: Experiments and Simulations*		
17:00 – 17:15	**Technical Talk 2**	**Wiley Publishers**		
17:15 – 18:35	***Parallel Session 1*** **Session Chair: Prof. A. Sen & Prof. J. Jose**		***Parallel Session 2*** **Session Chair: Prof. S. Mazumder & Prof. B. Goyal**	
17:15 – 17:35	**ST-3**	**Prof. Sandeep Nigam, BARC, Mumbai** *Computational Chemistry and Experiment: So Close, Yet So Far* *Sandeep Nigam*	**ST-7**	**Prof. Kailas D. Sonawane, Shivaji University, Kohlapur** *Understanding antibiotic resistance : A major public health problem*
17:35 – 17:55	**ST-4**	**Prof. Snehasis Daschakraborty, IIT Patna** *Photoswitchable Lipids in Liposomal Membrane: From Fundamentals to Applications*	**ST-8**	**Prof. G. Gopakumar, IGCAR, Kaplakkam** *Density Functional Theory Studies on the Separation and Recovery of Lanthanides and Actinides*
17:55 – 18:15	**ST-5**	**Prof. Divya Nayar, IIT Delhi** *Living Cell Soup: Biomolecular Self-Assembly to Nanomaterial Design*	**ST-9**	**Prof. Paritosh Modak, BARC, Mumbai** *Elemental Solids under High Pressure: A Case Study on Elemental Calcium*
18:15 – 18:35	**ST-6**	**Shri Pritam P. Shete, BARC, Mumbai** *Introduction to Large Language Models: From Foundation to Real World Applications*	**ST-10**	**Prof. Neetu Goel, Punjab University** *First Principle Tailoring of Metal Porphyrins for Electrocatalysis*
18:35 –18:45	**Tea Break**			
18:45 – 19:30	**Cultural Programme**			
19:30 Onwards	**Dinner**			

Day -3, 28th September 2024 (Saturday)

Time				
09:30 – 11:40	*Session 7* Session Chair: Prof. T. K. Ghanty			
09:30 – 10:00	Perspective Talk – 17	**Prof. R. B. Sunoj, IIT Bombay** *Molecular Machine Learning Approaches to Chemical Catalysis*		
10:00 – 10:30	Perspective Talk – 18	**Prof. Deva Priyakumar, IIIT Hyderabad** *Generative Artificial Intelligence in Molecular Science Research*		
10:30 – 11:00	Perspective Talk – 19	**Prof. Ram K. Roy , BITS-Pilani** *In Search of Mechanism of Aggregation Induced Emission: A Theoretical Study*		
11:00 – 10:20	ST-11	**Prof. Biswarup Pathak, IIT Indore** *Development of Artificially Intelligent Nanopores for HighThroughput Seque*		
11:20 – 11:40	ST-12	**Prof. Arnab Mukherjee, IISER Pune** *Reinforcement Learning Helix Disrupting Mutation*		
11:40 – 11:55	***Tea Break***			
11:55 – 12:55	*Parallel Session 3* Session Chair: Shri K. Bhanja & Prof. M. K. Ravva		*Parallel Session 4* Session Chair: Prof. M. Manna & Prof. A. Chand	
11:55 – 12:10	LT-2	**Prof. Achintya K. Dutta, IIT Bombay** *Relativistic Coupled Cluster Method Beyond Diatomic Molecules*	LT-6	**Prof. Padmesh A., IIT Palakkad** *Sub-Pico-Newton Forces and The Folding-Unfolding of Trpzip2 B-Hairpin*
12:10 – 12:25	LT-3	**Prof. Kaushik Talukdar, Bhattadev University, Bajali** *Relativistic Coupled-Cluster Study of Molecules for Precision Experiments*	LT-7	**Prof. Mudit Dixit, CLRI, Chennai** *Accelerating Materials Discovery for Catalysis and Electrochemical Energy Storage*
12:25 – 12:40	LT-4	**Prof. Prakash M. SRM University, Chennai** *Electrode/Electrolyte-Based Interface Models for CO2 Catalysis: A First Principle Study*	LT-8	**Prof. Brindaban Modak, BARC, Mumbai** *Tuning Intrinsic Defects through Dopant Engineering*
12:40 – 12:55	LT-5	**Prof. Tijo J. Vazhappilly, BARC, Mumbai** *Computational Modeling Of Materials for Energy Applications*	LT-9	**Prof. Harish Srinivasan, BARC, Mumbai** *Modeling, Theory, And Simulation in Soft Condensed Matter (F) Nature of Universal Subdiffusion Crossover in Molecular Glass-Formers*
12:55 – 13:40	**Lunch Break**			
13:40 – 15:10	*Session* : Poster Session & Tea (Categories: G-J) Session Chairs: Prof. H. P. Upadhyaya & Prof. A. K. Pathak (Members: Profs. R. Mishra, M. Pai, S. Varma, M. Kumbhakar, R. Ganguly, P. Mathi, A. Sen, M. Manna, S. Mahesh, Tijo J.)			
15:10 – 16:55	*Session 8* Session Chair: Prof. Chandra N. Patra & Prof. N. Choudhury			
15:10 – 15:40	Perspective Talk – 20	**Prof. Gopalan Rajaraman, IIT Bombay** *Role of Molecular Modelling in the Design and Development of Molecular Nano Magnets*		
15:40 – 16:10	Perspective Talk – 21	**Prof. Ranjan Mittal, BARC, Mumbai** *Phonons and Thermodynamic Behaviour of Novel Compounds: A Perspective from Neutron Scattering Experiments and Ab-initio Simulations*		
16:10 – 16:40	Perspective Talk – 22	**Prof. Rajarshi Chakrabarti, IIT Bombay** *Phase separation in active systems: insights from computer simulations*		
16:40 – 16:55	Technical Talk 3	**ACS Publishers**		
16:55 – 17:40	***Poster Awards & Concluding Session***			
19:30 Onwards	***Dinner***			

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Short Talks

Lightning Talks

D: Computational Chemistry Related to New Generation Nuclear Fuels

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I: Experiment Driven Theoretical Investigations

J: Modeling, Theory and Simulation for the Exploration of Biological Phenomena and Drug Design

Plenary Lectures

PL-1

Accurate methods for shape resonance and decay processes in molecules

Sourav Pal
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This talk will present highly precise coupled cluster formalism using complex absorbing potential (CAP), which makes the decay and resonant wave-functions square-integrable. Thus, accurate bound state methods like multi-reference coupled cluster (MRCC) can be used for such properties. The talk will present our calculations of electron molecule resonance, auger and inter-atomic columbic decay, their widths using the appropriate versions of CAP-MRCC formalism developed by us and compare these with experimental numbers where available. Predictive scope of the method will be highlighted.

PL-2

Computational materials science and its applications in the area of materials for energy

Rajeev Ahuja[a,b]

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Energy storage has been a theme for scientists for two hundred years. The Lead acid battery research on batteries occupied some of the best minds of the 19th century. Gaston Plante in 1859 invented the lead acid battery which starts your car and ignites the internal combustion which takes over the propulsion. Although the lead battery is over 150 years old but the origin of its open circuit voltage (OCV) of 2.1 V is still known. In present talk, I will show how one can explain the origin of OCV of 2.1 V based on foundations of relativistic quantum mechanics. Surprisingly, seems to be the first time its chemistry has been theoretically modeled from the first principles of quantum mechanics. The main message of this work is that most of the electromotoric force (1.7-1.8 Volts out of 2.1 V) of the common lead battery comes from relativistic effects. While the importance of relativistic effects in heavy-element chemistry is well-known since over two decades, this is a striking example on "everyday relativity". We believe that the fact that "cars start due to relativity."

The purpose of this talk is to provide an overview of the most recent studies in the field of hydrogen storage materials & rechargeable battery research with the focus how computational material science can play an important role in search and design of new hydrogen storage materials & next generation battery materials. On specific examples, the application of density functional theory calculations and molecular dynamics simulations will be illustrated to show how these computational methods can be of great use in the effort to reach a better understanding of materials and to guide the search for new promising candidates.

PL-3

Memory Effects and Quantum Coherence in Excitation Energy Transfer in Photosynthetic Reaction Systems

Rajesh Dutta[a] and Biman Bagchi[b*]

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Fluctuations in the energy gap and coupling constants in and between chromophores can play important role in the absorption and energy transfer across a collection of two-level systems that often serve as theoretical models in photosynthetic reaction systems in a noisy environment, fluctuations can control efficiency of energy transfer through several factors, including quantum coherence. In photosynthesis, the role of light-induced quantum coherence on the efficiency of energy transfer to a designated "trap" state has been studied extensively. However, these studies have typically employed either a Markovian, or a perturbative approximation for the environment induced fluctuations. In this study, we depart from these approaches to incorporate memory effects by using Kubo's quantum stochastic Liouville equation (QSLE). We introduce the effects of the decay of excitation (to the ground state) and the desired trapping that provides the direction of the motion of the excitation. In the presence of light-induced pumping, we establish a relation between the mean survival time, efficiency, and the correlation decay time of the bath-induced fluctuations. We recover a connection between transfer flux and the imaginary part of coherences in both equilibrium and excited bath states, in both correlated and uncorrelated bath models. We uncover a non-monotonic dependence of efficiency on site energy heterogeneity for both correlated and uncorrelated bath models.

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Perspective Talks

PT-1

2-TIPS and ordering in various active matter systems

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2-TIPS (Two Temperature induced phase separation) refers to the phase separation phenomenon observed in mixtures of active and passive particles which are modelled using scalar activity. Scalar activity was introduced by increasing the temperature of half of particles (labeled ‘hot’) while keeping the temperature of the other half constant at a lower value (labelled ‘cold’). The relative temperature difference between the two subsystems is considered as a measure of the activity. We report 2-TIPS and crystallization in a system of 3-d LJ particles taken at state points spanning from gas to liquid regime using Molecular dynamics simulation (MD). From our simulations we observe that the two species tend to phase separate at sufficiently high activity ratio. We observe similar activity induced phase separation in a mixture of active and passive dumbbells. We also study the order-disorder transition and phase separation in a mixture of hot and cold spherocylinder of different aspect ratio (L/D) interacting through Weeks-Chandler-Anderson (WCA) potential in three dimensions. Activity drives the cold particles through a phase transition to a more ordered liquid crystalline (LC) state and the hot particles to a state of less order compared to the initial equilibrium state. The cold components of a homogeneous isotropic (I) structure acquire nematic (N) and, at higher activity, crystalline (K) order. Similarly, the cold zone of a nematic initial state undergoes smectic (Sm) and crystal ordering above a critical value of activity while the hot component turns isotropic. Surprisingly, activity induces LC ordering for spherocylinder having aspect ratio below Onsager limit. We find that the hot particles occupy a larger volume and exert an extra kinetic pressure, confining, compressing and provoking an ordering transition of the cold-particle domains. Finally, we show similar activity induced phase separation in a chiral system.

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5. Effect of Confinement and Topology: 2-TIPS vs MIPS, Nayana Venkatareddy, Jaydeep Mandal, Prabal K. Maiti, Soft Matter (2023)

PT-2

Interfacial Properties of Biomolecules in Aqueous Ionic Liquid Solutions

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Structural stabilities and activities of biomolecular systems, such as proteins, nucleic acids, lipid membranes are known to be sensitive to the presence of ionic liquids (ILs) as co-solvents in aqueous media. To obtain a generic understanding of the mechanism of action of ILs on proteins,it is important to elucidate protein-IL interaction and probe the modified interfacial environment around proteins in binary water-IL solutions containing ILs with different cation-anion combinations. We have carried out extensive molecular dynamics (MD) simulations of a series of amino acids [1] and proteins in different aqueous IL solutions [2-8]. Preferential distribution of the IL components at the interface with replacement of water molecules, and their non-uniform influence on the interfacial properties have been explored in detail. Attempts have also been made to explore the effects of ILs on the structure, stability and interfacial properties of phospholipid bilayers and DNAs. Several important findings originating from our studies will be presented.

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PT-3

Efficient screening of single phase forming low-activation high entropy alloys

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In traditional alloy design, one or two primary elements are alloyed with minor auxiliary elements. High entropy alloys (HEAs), as opposed to ordinary alloys, mix four or more elements at equal or almost equal proportions, frequently in a single crystalline phase. High configurational entropy has been linked to, among other crucial aspects, the rather exceptional stabilization of multicomponent alloys in a single phase against the production of numerous phases and intermetallics. A remarkable combination of strength and ductility, high damage tolerance, excellent corrosion resistance, exceptional fracture toughness at cryogenic temperatures, etc., are some of the promising properties to offer by HEAs.

For a material to function in harsh Gen-IV fission/fusion nuclear reactor conditions, one of the critical requirements is that after exposure to energetic neutrons, the radioactivity of the employed elements should decay quickly to low levels in a time scale of fewer than 100 years. The talk will discuss efficient screening of chemical space constituting a palette of seven low-activation metallic elements (Ti, V, Cr, Mn, Fe, Ta, and W) to find a single-phase equiatomic/non-equiatomic body-centered cubic (BCC) quaternary/quinary high entropy alloys (HEA). A high throughput screening using ab-initio computations-assisted thermodynamic modeling strategy will be discussed. Benchmarking the accuracies of the empirical models for predicting simple solid solutions HEAs is performed and based on the most efficient empirical model and employing machine-learning, compositional ranges of several new single-phase forming HEAs are suggested. A thorough comparison of high-throughput screening results with CALPHAD data and experiments establishes the efficiency of the high-throughput screening strategy.

PT-4

Exploration of Free Energy Landscape of Complex Molecular Systems: Dynamics to Thermodynamics and Back

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Understanding the molecular mechanism of any complex biophysical or chemical processes requires tracking of the dynamics on the underlying (free) energy landscape. For all practical purposes, this requires projection from a higher dimensional landscape (3N for N particle system) onto a few collective variables or order parameters or reaction coordinates. The accuracy of the computed free energy landscape or kinetic parameters often strongly depends on this choice of collective variables to project on. In this talk, we shall discuss a few representative case studies to elucidate the complexity or difficulty of this choice. We shall discuss classic order parameters based on chemical or physical intuition along with machine learned (artificial neural network based) reaction coordinates for complex processes where intuition may fail.

We shall also discuss an ongoing development of a weighted ensemble based enhanced sampling method to quantitatively estimate kinetics of rare events, e.g. protein unfolding or ligand unbinding.

PT-5

Hydration of metal ions and molecules

Dilip. K. Maity

Bhabha Atomic Research Centre, Mumbai & Homi Bhabha National Institute, Mumbai

Metal ion-water and neutral or charged molecule-water binding are continued to be an important research topic not only in the fields of chemical, physical or biological sciences but also for the efficient development of separation processes. The spatial distribution of water molecules around a metal cation commonly follows symmetric pattern that in turn minimizes the water-water interactions. However, in case of molecular systems, the distribution of solvent water molecules varies depending on strength of hydrogen bonds formed between an active site of molecular system and solvent water molecules. Hydration may lead to dissociation of certain class of molecules and may facilitate proton transfer in many molecular systems including biological systems.

In this talk, we plan to discuss hydration of metal cations and a selected class of molecular systems and its manifestation in different molecular properties.

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PT-6

Quo Vadis DFT: a Perspective

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Versatility in handling various condensed systems, flexibility of improvements and refinements, amenability to meaningful extensions, possibility of adding higher levels of complexity, etc. are some of the unique combinations of characteristics that have made DFT the primary computational tool for understanding as well as predicting the physical and chemical properties of a wide variety of materials from bulk to nano, and also in designing novel materials with desired combination of properties. The precision with which one can estimate these properties, as well as their accuracy to validate with the corresponding experimental results, have been extensively studied. While this approach has proved very useful, computational scaling limits their applicability to relatively smaller systems (~100s of atoms). With the advent of exa-scale computing facilities with massively parallel architecture, there have been attempts to use non-conventional basis-sets as well as order-N approaches to venture into large scale problems with direct practical implications.

In this talk, I shall attempt to provide a perspective of some of the methodological developments, followed by a few examples of large nano-clusters and complex interfaces that we have investigated in the recent past. I shall end my talk with the possible challenges and limitations being faced by the community and some possible ways to overcoming these.

PT-7

Global Optimization of Atomic Clusters: A Soft Computing Perspective

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Geometry optimization of chemical systems like atomic clusters becomes a daunting task because of the large size of the search space and the possibility of getting stuck in a local minimum on the potential energy surface. Determination of global minimum energy structure needs the gradient and Hessian matrices to be calculated at each stage and with no guarantee of locating the global minimum. Various soft computing techniques may be made use of, bypassing this hassle. We present methods like particles warm optimization combined with density functional theory, atom centered density matrix propagation and convolutional neural network and also a firefly algorithm for global optimization of atomic clusters. We highlight their efficiency and accuracy by considering different metallic and non-metallic clusters as prototype examples. A comparison is made regarding the efficacy of these algorithms vis-à-vis other standard machine learning methods like simulated annealing, basin hopping, artificial bee colony and Bonobo algorithms.

PT-8

A new approach to a Generalized Smoluchowski Equation

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A unified approach [1] for deriving an exact kinetic equation for the distribution function of an arbitrary phase space function of a many-body system is presented. A rigorous derivation of the kinetic equation for unreactive as well as reactive situations is accomplished, by starting from the Liouvillie's equation. We consider a many particle system which at an initial time (t=0) is prepared in a constrained equilibrium state. The Effect of the constraint on the distribution function is discussed. We also point out how these results will be used for application [2-6]. The kinetic equation for classical density functional equation is also derived.

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PT-9

Large Molecules in Solution: Multiscale Modeling and Simulation

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Understanding the behavior of large molecules in solution is a long-standing problem in chemical physics as it defines the very basics of interactions at different length and time scales. The many-body nature of these interactions that includes correlated solvent motions, poses a serious challenge for the development of an analytic theory. The present talk will emphasize three specific application areas, viz. (a) the behavior of room temperature ionic liquids (RTILs) in different molecular solvents, (b) the structure of polymers at different interfaces, and (c) overcharging and charge reversals for a colloidal macromolecule in a spherical double layer environment.

The first application involves a hybrid simulation method involving RTIL-solvent system, where the solvent is modeled via LB with fluctuating stress tensor and a MD simulation for the RTIL molecules. The method is found to be quite successful in predicting the physical properties that agree well with the experimental results. The second area entails the amalgamation of Monte Carlo simulation and density functional theory for polymers, that is able to reproduce quite accurately the structural features of polymer molecules with complex architectures.[1] The third application involves combining the integral equation theory of uniform fluids to that of density functional theory of non uniform fluids, generating a self-consistent density-functional approach. [2] This has shown recent success in predicting the electrode-electrolyte interface beyond the primitive model for fully asymmetric electrolytes. [3] All the three application areas based the recent developments will be discussed along with a number of representative results.

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PT-10

The effect of surface temperature on molecule-surface scattering processes

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The studies on molecule-surface scattering processes have enormous importance in understanding the heterogeneous catalytic reactions. The effect of surface mode vibrations and their state distribution at a specific surface temperature for H_2/D_2-Cu(111) dissociative chemisorptions systems is explored for those molecules in their rovibrational ground state (v=0, j=0). We assume weakly correlated interactions between molecular degrees of freedom (DOFs) and surface vibrational modes through a Hartree product type wavefunction [1] within the linear and bilinear (anharmonic) molecular DOFs-surface modes coupling regime. While constructing the six-dimensional effective Hamiltonian, we employ (a) a chemically accurate potential energy surface according to the static corrugation model [2]; (b) normal mode frequencies and displacement vectors calculated with different surface potentials [3-5] within a cluster approximation; (c) slab models resulting in phonons at 0 and 925 K according to the quasi-harmonic approximation [6]; and (d) initial state distributions for the vibrational modes according to Bose–Einstein probability factors. We perform6D quantum dynamics [6-8] with the so-constructed effective Hamiltonian and calculate sticking and state-to-state scattering probabilities. As observed in experiments [9,10], surface mode vibrations significantly influence chemisorptions dynamics by exhibiting vibrational quantum effects and surface atom recoil effects at both low and high collision energies of the incoming diatom. Our current approach involves accurate phonon calculations including thermal lattice expansion and applying the correct Bose-Einstein statistics, which closely mimics the experimental conditions and provide more detailed mechanistic insights. Comparisons between our results, experimental data and other theoretical findings further demonstrate the novelty and effectiveness of our theoretical model [6,7,8,11].

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PT-11

Exploring Rugged Energy Landscapes of Enzymatic Reactions

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Exploration and computation of free energy surfaces of chemical reactions are pivotal to computationally predicting reaction mechanisms, pathways, and kinetics. Computing free energy surfaces of complex reactions, especially in soft matter systems, requires advanced molecular dynamics (MD) simulation techniques. Although tremendous progress has been made in recent years in this direction, several limitations are yet to be addressed to make the computations efficient and more accurate. Over the past few years, my group has proposed several new methods to address the outstanding challenges. In my talk, I will present some of our recent contributions in this area. In particular, I will demonstrate how the new methods and codes we developed can aid in developing new covalent inhibitors for beta-lactamase enzymes to compact antibiotic resistance.

PT-12

Terahertz Spectroscopy of Aqueous Systems using Polarizable Models

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Terahertz (THz) spectroscopy of water and aqueous ionic solutions in bulk and at surfaces are studied theoretically using polarizable models for both water and ions. The results are linked to underlying intermolecular interactions and dynamics. First, calculations are performed for pure water for varying temperature and the calculated results of THz spectroscopy are compared with experiments wherever available [1]. Subsequently, THz spectra are calculated for aqueous solutions containing alkali halide ions for different alkali and halide ions and the results are linked to various intermolecular interactions and dynamics of these solutions in the hydration shells [2]. Preliminary results will also be discussed for the second order THz spectroscopy of aqueous surfaces [3].

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PT-13

Optimizing Collective Variable for Linear Hydrophobic Polymer Collapse and Protein Folding Transitions: Crucial Role of Hydration

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Choosing appropriate collective variable for bio-molecular processes is a challenging task. Moreover, while constructing the free energy landscape of flexible biomolecules, solvent degree of freedom is often neglected to reduce the computational burden. In this work, we construct the optimized collective variable for different lengths of linear n-alkane chains by employing time-structured independent component analysis (TICA) framework as a linear combination of multiple order parameters (OPs) including the number of first hydration layer water molecules as a collective variable. The optimized collective variable from TICA successfully resolved the whole free energy landscape connecting different basins of polymer chain. We have found that Rg and end-to-end distance are the two important order parameters for these systems. Moreover, end-to-end distance is necessary to capture the crucial intermediate state present along the transition pathway. We have constructed markov state model (MSM) to find out different kinetic pathways connecting different metastable basins. In this work, we have proposed one protocol to quantitatively identify the contribution of different OPs specifically in the transition state ensembles (TSE) through XGBoost model in conjuncture with explainable AI algorithm Shapley Additive explanation (SHAP). Interestingly, we have found that hydration water is the most crucial order parameter near the major barrier going from extended to intermediate state, where a send-to-end distance is important for the secondary barrier going from intermediate to collapsed state [1]. We further extend this protocol to find out the optimized reaction coordinate in protein folding transition. We have developed a neural network architecture based on denoising integrated auto encoder framework incorporating time-lag information to accuratelycapture the system's kineticsand to separate multiple low populated metastable basins present in the free energy landscape. We have chosen two small protein system: a mutant of chignolin (10 residue) and Trp-cage (20 residue) and shown that our method identified multiple metastable basins in the landscape including the misfolded conformations, consistent with NMR studies. We have also found folding and unfolding times calculated from MSM shows close resembles with experiments. Moreover, using the proposed protocol of analyzing contribution of OPs in the TSE, we have found that hydration water is important OP near the major barrier for this system which essentially means that desolvation of water molecules from the core is the slowest step. Overall, our study provides a flexible route to find out the important order parameters in the TSE which can be applied for even complex biomolecular systems.

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PT-14

Liquid Phase of Deep Eutectics: Enthalpy versus Entropy

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Enthalpy or entropy – which one is the key for accessing the liquid phase of deep eutectics composed of room temperature solid components? This is an important question which has not been thoroughly investigated yet and thus remained ill-understood. The easy tunability of physicochemical properties of DESs, low cost and relatively lower impact on environment have made these solvents quite popular as reaction media in chemical industries[1]. Several model approaches, such as, the regular solution theory and the Flory-Huggins theory, attempted to parameterize the non-ideality of molten mixtures in order to connect to the depression of the freezing point[2] but did not provide any framework to consistently incorporate inter-particle interactions in the enthalpy and entropy contributions to the over-all changes in the Gibb's free energy of mixing[3].We have developed a theoretical schemewhich systemically incorporates the interparticle interactions for the calculations of both the enthalpic and entropic contributions and provide a clear thermodynamic explanation for stabilisation of the liquid phase at the deep eutectic condition for a given mixture. Enthalpic contributions to the change in free energy has been obtained from molecular dynamics simulations through counting of interparticle interactions, while the 2PT method[4] has been employed to estimate the corresponding entropic contribution. The robustness of our theory has been verified by successfully predicting the melting temperatures of a few known mixtures. Our theory suggests that a novel interplay between the enthalpic and the entropic contributions govern the accessibility of the liquid phase and the nature of the inter-species interactions decides the dominance of one of them over the other.

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PT-15

Dehydration Induced Selective Ion Trapping by Topology Constrained Atomically Thin Graphene-Crown Membranes

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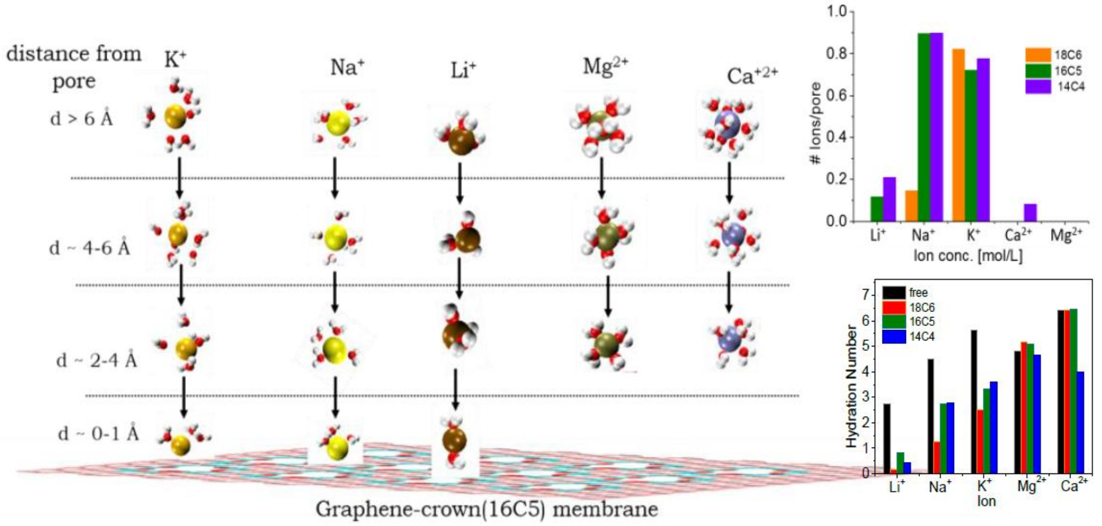
Development of a suitable nanomaterial for the regulation of ion transport has been a longstanding topic to tune ion sensing and transport across nanoscale pores. Computationally designed membrane employing molecular dynamics and density functional theoretical simulations are quite well accepted for understanding the ionic transport through nanoscale pores and hence can be used as a complimentary tool to complex experiments like nanofluidics logical devices. In that perspective, robust MD simulations and DFT calculations were conducted to investigate the selective capturing of metal ions by graphene-embedded 18-crown-6, 16-crown-5 and 14-crown-4. Spontaneous and stable trapping of metal ions with different graphene-crown membrane demonstrated the utilization of these graphene-crown membranes for nanofluidics logical devices. The present systems can be utilized as highly sensitive platform for micro-solvation studies and open the secret that why one would feel momentous differences in ionic conductivity with adsorption of particular ionic species. The present talk will cover the atomistic findings which might open up new era in gas sensing, ion separation, energy storage, drug delivery, nanofluidics logical devices, and devising of ion-channel-inspired materials using hybrid graphene-crown membranes.



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PT-16

Unusual Dynamics, Phase Behavior and Yielding of Dense Stimuli Responsive Microgel Glasses: Experiments and Simulations

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Poly (N-isopropylacrylamide) (PNIPAM) microgel particles are soft spheres with a core-shell structure having a dense polymer core and thin shell consisting of less cross-linked polymers and dangling polymer chains (hairs). Dense suspensions of these hairy soft-spheres exhibit structural ordering similar to that observed in atomic systems. Ordered structures of these microgel suspensions exhibit series of phase transitions with increase in temperature and osmotic pressure. In this talk I will present results obtained by performing investigations using static and dynamic light scattering, UV-Visible spectroscopy and rheology results on ordered (crystalline) and disordered (glassy) structures of thermo-responsive and pH responsive microgel suspensions with volume fractions, $\phi < 0.74$ and under over packed ($\phi > 0.74$) conditions. Under over packed conditions we show that these soft spheres undergo deswelling and exhibit unusual dynamics at short times. The talk presents three surprising results on PNIPAM microgel suspensions under over packed conditions: (i) observation of stable FCC-HCP coexistence in microgel crystals (ii) two step yielding in microgel glasses and (iii) Sub-diffusive behavior at short-time scales. The entanglement of hairs between neighboring soft-spheres under over packed conditions are shown to be responsible for the above mentioned results. To provide an unambiguous evidence in favor of existence of entanglements, we prepared microgel particle without hairs, i.e. particles having only homogeneous polymer core. Non-linear rheological studies and dynamic light scattering measurements on a dense glassy sample indeed showed only single step yielding and absence of sub-diffusive behavior at short times, respectively. These observations constitute evidence in favor of presence of entanglements between hairs and understanding for the unusual behavior of dense microgel crystals and glasses of core-shell structured stimuli responsive microgel particles. Monte Carlo (MC) and Oscillatory Shear Simulations have been carried out with an effect pair-potential proposed by Maxime J. Bergman et al. [Nat. Commun. 9, 5039 (2018)] for colloidal PNIPAM microgels. The talk presents the inadequacy of this pair-potential (U(r)) and the need for an additional hair-term in U(r) to understand the above mentioned experimental observations over a wide range of volume fractions.

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PT-17

Molecular Machine Learning Approaches to Chemical Catalysis

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PT-18

Generative Artificial Intelligence in Molecular Science Research

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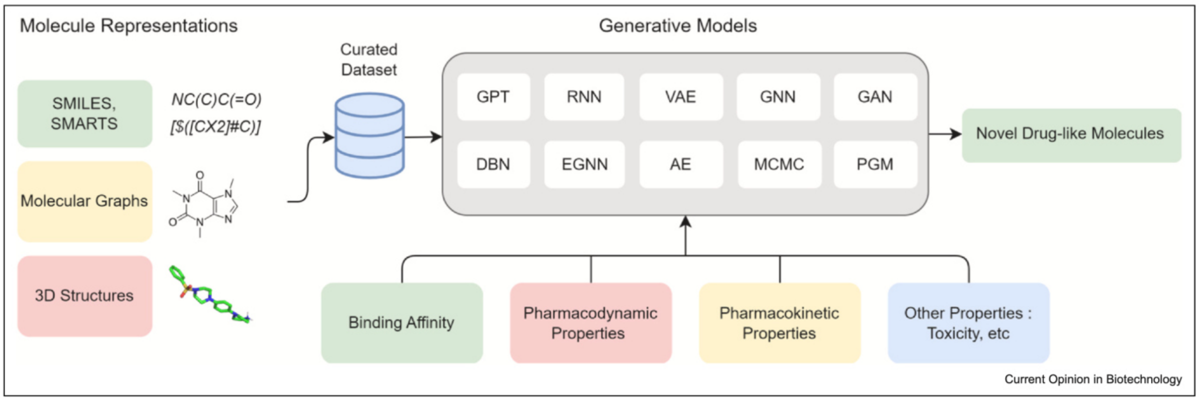
Generative AI (or GenAI), a short of Generative Artificial Intelligence, is a subset of artificial intelligence that creates new data resembling a given dataset instead of merely recognizing patterns or making predictions. These models learn the data's underlying structure to produce novel, synthetic examples, rather than direct copies, accelerating innovation across various domains. Techniques like generative adversarial networks (GANs), variational autoencoders (VAEs), transformers, and reinforcement learning have diverse applications, including drug discovery.

In this talk, we will discuss the use of variational autoencoder for generating inorganic materials with desired properties as a proof of concept. We use a simple one-hot encoding for representing inorganic molecules based on which a generative model is trained. A series of tests were done to examine the robustness of the predictor models, to demonstrate the continuity of the latent material space, and its ability to generate materials exhibiting target property values. Following this, we will discuss the use of recurrent neural network assisted by reinforcement learning for generating drug like molecules with desired physico-chemical properties and binding affinity with respect to select targets. Generative pretrained models (such as ChatGPT) have had phenomenal success in generating textual content during the last few years. We have trained a GPT architecture that is capable of generating valid and novel molecules initially. This model is further trained to suggest molecules that possess desired properties such as LogP, QED, solubility, etc. As the next step, in order to generate molecules with more complex properties, we use direct preference optimization along with GPT to show that our model, MolGPT, is able to propose novel molecules that strongly bind with specific drug targets.



Current Opinion in Biotechnology

Figure 1. Schematic representation of a typical generative AI pipeline for molecular/material design.

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PT-19

In Search of Mechanism of Aggregation Induced Emission: A Theoretical Study

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The aggregation-induced emission (AIE) mechanism of the fluorescent styrene derivative 4-dimethylamino-2-benzylidene malonic acid dimethyl ester (BIM) in methanol solution is theoretically investigated using spin-flip [1] long-range corrected [2, 3] time-dependent density functional theory. Our calculation reveals that there is nearly 77-degrees variation in the α angle (due to rotation around the aryl main axis) as we move from S_0 optimized state to the S_1 optimized state, which is perfectly consistent with experimental observations. Subsequently, the potential energy surfaces (PESs) for the ground (S_0) and the first singlet excited (S_1) states of BIM were generated along the rotation of the aryl main axis (i.e., α angle rotation) [4]. For the monomer, our findings reveal a significant reduction in oscillator strength, approaching zero at the optimized geometry in the S_1 state. As this state corresponds to a charge transfer state, it suggests that the BIM monomer operates as a twisted intramolecular charge transfer (TICT) system, undergoing quenching through α angle rotation. The PES scan for the S_0 and S_1 states of the BIM dimer, which serves as a model for the aggregate state, is also being carried out. The initial results indicate an increase in oscillator strength value, $f = 1.08$ a.u., and the restriction of α angle rotation at the S_1 optimized geometry compared to that of the monomer. These findings lead to the conclusion that the AIE mechanism of BIM is driven by TICT-induced quenching of fluorescence in the monomer and the absence of the same in the dimer (a miniature prototype of the aggregate state) due to inhibition of synchronous α and γ angle rotation.

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PT-20

Role of Molecular Modelling in the Design and Development of Molecular Nano Magnets

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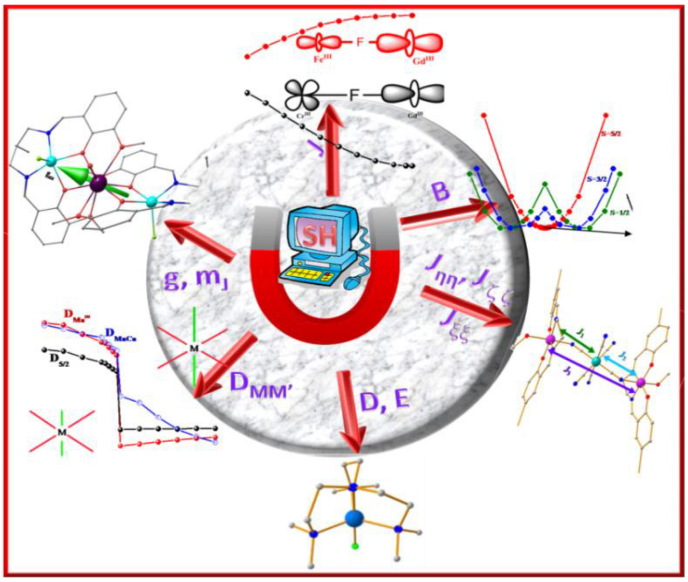
Molecular magnetism is one of the vastly growing research fields with an aim to design molecules and materials with tunable magnetic and electronic properties.**Error! Reference source not found.** Their synthesis, characterization and implementation as devices create a lively crossroad among chemistry, physics and material science: a multidisciplinary research field. These molecules have widespread potential applications ranging from magnetic storage devices, spintronics, and Q-bits in quantum computing to magnetic coolants.**Error! Reference source not found.** Single-molecule magnets (SMMs) are the molecules which show slow relaxation of magnetization below the critical temperature and exhibit a hysteresis loop similar to classical magnets. SMMs offer key advantages over classical magnets due to their lightweight, solubility and multifunctional behaviour. Theoretical tools are indispensable in this arena[2] for understanding the observed magnetic properties. The strength of these methods is not only limited rationalization but also the prediction of novel molecules which can exhibit superior magnetic properties. In this presentation, I will research the effort undertaken by our group towards achieving this goal.[2, 3]



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PT-21

Phonons and Thermodynamic Behaviour of Novel Compounds: A Perspective from Neutron Scattering Experiments and Ab-initio Simulations

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Inelastic neutron scattering is widely used for the measurements of phonon dispersion relation and phonon density of states in polycrystalline and amorphous solids in various materials. We have been extensively using the inelastic neutron scattering and lattice dynamics simulations to study the phonon properties of novel compounds. Few examples [1-4] from our recent studies will be discussed in this talk.

Work on anomalous thermal expansion compounds provides a microscopic understanding of the underlying mechanism. Our studies of the ionic diffusion in Li/Na solid state battery materials, have focused on the important role of soft-phonons, besides the structural and compositional features such as defects, amorphization, and stoichiometry. We showedthat the coupling of the dynamics of Li ion with its neighboring SiO_4 polyhedral units in the amorphous phase of $Li_2Si_2O_5$ helps to accelerate the Li^+ diffusion. In case of Na_3ZnGaX_4 (X=S, and Se), we have shown that the specific topology of the crystal structure provides clear zig-zag highways for Na-ion diffusion. These highways comprise of low-potential energy positions of the Na-atoms connected by low-energy barriers for diffusion.

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PT-22

Phase separation in active systems: insights from computer simulations

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To understand the motion of active shape- deforming agents,a collection of rings made of active Brownian particles (ABPs) [1, 2] for different packing fractions and activities is investigate dusing computer simulations. Our computer simulations reveal that active rings display an ovel dynamic clustering [3] instead of the conventional motility- induced phase separation (MIPS) [4] as observed in case of collection of ABPs. Surprisingly, increasing packing fraction of rings exhibits a non-monotonicity in the dynamics due to the formation of a large number of small clusters. The conformational fluctuations of the polymers suppress MIPS exhibited by ABPs. This demonstrates a complex interplay between activity, topology, and connectivity.

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Short Talks

ST-01

Uranyl Ion Binding to Human Serum Albumin: Influence of Fatty Acid

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Actinides are regularly encountered in various stages of the nuclear fuel cycle, and even with stringent safety criteria and several radiation safeguards in place, the potential for internal contamination from these actinides should not be ignored. Investigations into the interactions of actinides with the body fluids in living organisms are essential in order to understand and minimise the possible health risks. Human serum albumin (HSA), the most abundant plasma protein, may play a key role in these interactions. Distinct binding behaviours of zinc and uranyl ions with HSA are observed, and their interactions are influenced by the presence of fatty acids [1-2]. The binding behaviours are investigated by analysing hydrogen bond dynamics, short-range interactions, and by constructing the potential of mean force profiles. Present results may open up a new window for further exploration of actinide interaction with body fluids and potential applications in the development of decorporating agents for actinide contamination.

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ST-02

Theory Driven Experiments for Small Molecule Activation

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Small-molecule activation has garnered significant interest in converting them into value-added chemicals. Host-guest supramolecular chemistry offers a promising approach for facilitating such activation. Cucurbiturils (CB[n]) are known for their exceptional encapsulation abilities and are an ideal choice for enabling efficient small-molecule activation. Using high-valent Fe^{IV}=O species strapped to CB [5] is highly effective for activating C-H bonds, including methane. Understanding the kinetics and thermodynamics of encapsulation is crucial for supramolecular catalysis. We have investigated various simple alkane encapsulation to CB-[6] cavity. Ni-Cyclam, a widely recognized CO2 reduction catalyst, is investigated here to explore its catalytic performance upon encapsulation with CB [8]. We will discuss these new results in this presentation.

ST-03

Computational Chemistry and Experiment: So Close, Yet So Far

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Computational materials chemistry fortifies a broad spectrum of science disciplines, including basic chemistry, catalysis, nano-science, materials science, environmental science, geosciences and renewable energy. Computational studies have been indispensable tool to get insight regarding origins of chemical phenomena and examination of physicochemical properties. Sometimes experiments are expensive and time-consuming, materials scientists have been relying on computational methods for computation of materials properties and processes at the atomic level to guide/support experiments. However, close mimicking the experimental conditions has been a challenge for computational chemistry. The present talk will be providing summary of our recent joint computational and experimental efforts for designing materials for energy applications. The talk will accentuate on challenges of gelling computational & experimental investigations and subsequently achieving the coherence between the two investigations for meaningful scientific conclusion.

ST-04

Photoswitchable Lipids in Liposomal Membrane: From Fundamentals to Applications

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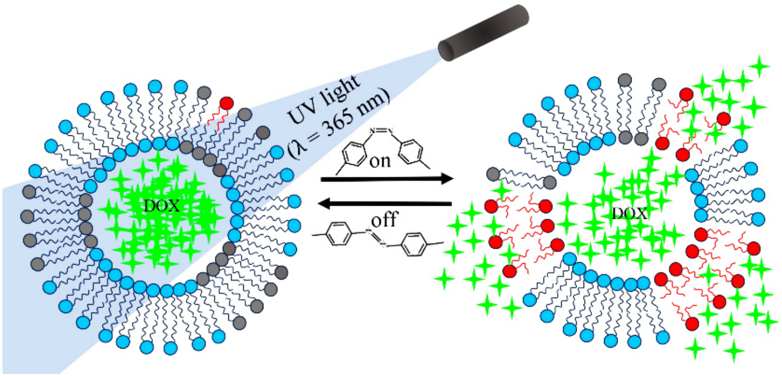
In this talk, I will explore the molecular-level impact of photo-isomerization on membrane structure and dynamics, specifically focusing on lipids containing azobenzene groups (PSLs) within their acyl chains. Using all-atom molecular dynamics simulations, we investigate how UV-induced trans-to-cis isomerization of azobenzene-derivatized phosphatidylcholine (AzoPC) lipids affects the structure and dynamics of a model lipid membrane, mimicking E. coli bacteria at various temperatures. Our findings not only corroborate experimental observations of membrane properties but also shed light on localized effects and microscopic heterogeneity within the membrane. Furthermore, I will discuss our estimation of the relaxation timescale of the lipid membrane post-AzoPC photo-isomerization. Lastly, I will present our demonstration of photo-activated drug release, using doxorubicin as a model, and highlight the potential of PSLs in designing photo-activated liposomes, or photoazosomes, for precise and targeted drug delivery applications.



ST-05

Living Cell Soup: Biomolecular Self-Assembly to Nanomaterial Design

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Biomolecules evolve and function inside a crowded intracellular environment. The living cell milieu is tightly packed with high concentrations of macromolecules, small cosolutes, ions and restricted water.[1] This tight packing exerts crowding effects that are expected to crucially modulate biomolecular structure and dynamics. Although these effects had been identified in 1958,[2] they have yet remained under-appreciated and a comprehensive molecular-level understanding has remained inconclusive. The traditional view of crowding highlights that crowded milieu induces compaction in biomolecules via entropic effects.[1,2] The new view indicates that the crowded environment may either promote or oppose biomolecular collapse and the soft interactions can play a crucial role in these processes.[3-5] Moreover, crowding has attracted applications in nanomaterial design for therapeutics and biodiagnostics. It can be used as a tool to design self-assembly of bio-functionalized metal nanoparticles with tuneable properties. The talk will address the following questions: (a) does a crowded environment always lead to self-assembly or collapse of biomolecules? (b) can we understand the role of intermolecular attractions in a more explicit way? (c) what are the thermodynamic driving forces underlying such effects? (d) can the current molecular simulation models accurately model a crowded environment?[6] An overview of molecular understanding of crowding effects will be provided for the self-assembly and salvation of interesting systems such as of amyloid oligomers, responsive polymers and ss-DNA capped gold nanoparticles.

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ST-06

Introduction to Large Language Models: From Foundation to Real World Applications

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Large Language Models (LLMs) have transformed the field of Natural Language Processing (NLP). The invited talk will introduce the fundamentals of LLMs and explore their practical applications in the real world. LLMs are pre-trained on extensive datasets derived from publicly available sources to grasp semantics of language. These are then further fine-tuned on specific tasks, such as text summarization, machine translation, and sentiment analysis and are continuously monitored and refined through human feedback for aligning them with human values and performance improvements. After a brief introduction to LLMs, the talk will quickly glance through numerous applications of LLMs across various industries and domains. Then the talk will cover applications specific to the research community. LLMs summarize long pieces of text into concise summaries, making it easier to understand complex information which is essential for research work. LLMs are generating high-quality articles saving time and effort for content creators. Then the talk will go deeper into our own experiences in BARC for designing and developing LLM based applications. LLM based Retrieval Augmented Generation (RAG) answers questions based on a large corpus of text, making it a useful tool for research and knowledge discovery. The talk will cover design and development of in-house Sahaayak system, which is a RAG based Interactive Q&A system for precisely answering queries on private BARC documents. Lastly, the talk will provide infrastructure required for deploying, fine-tuning, and training LLMs with the help of the in-house Pragya infrastructure, which is dedicated for machine learning applications.

ST-07

Understanding antibiotic resistance: A major public health problem

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Global emergence of antimicrobial resistance, combined with the current COVID-19 pandemic, highlight the need for action plans for better treatment of infectious microorganisms. One of the biggest global public health issues of our time is antibiotic resistance, which is the ability of microbes to resist drugs meant to kill them. The antibiotic resistant bacteria and biofilm forming bacteria, make treatment less effective against various infections. One of the most important strategies in the fight against AMR is the search for new antibiotic classes. Over the last decade, there has been a dramatic increase in the number of computational applications and tools developed to help researchers more efficiently carry out modern drug discovery programs. Understanding bacterial resistance at the atomic level could help in the development of new inhibitors for resistant pathogens. Bacterial resistance to aminoglycoside antibiotics is primarily caused by aminoglycoside phosphotransferases (APHs). Thus, we used homology modelling, molecular docking, molecular dynamics (MD) simulation, and principal component analysis to understand structural significance of APH from *B. cereus.* Molecular docking and MD simulation were helpful to investigate the mechanism of substrate and inhibitor binding to APH, which revealed that GTP was the preferred substrate and ZINC71575479 was the most effective inhibitor. Similarly, a comprehensive structural analysis of dipeptide modifying D-Alanine: D-Serine ligase (Ddls) was carried out to screen its inhibitors for combating vancomycin resistance. In this study, modeled 3D structure of EgDdls from *E. gallinarum* was used for structure-based virtual screening (SBVS) of oxadiazole derivatives. Hence, computational studies of antibiotic resistance mechanisms and structure-based virtual screening could be beneficial to design new drug molecules.

Keywords: Antibiotic resistance, Homology modelling, Molecular docking, Molecular dynamics simulation

ST-08

Density Functional Theory Studies on the Separation and Recovery of Lanthanides and Actinides

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Actinide separation and recovery is important at various stages of nuclear fuel cycle. The recovery of uranium and plutonium from the spent fuel is a vital step in the nuclear fuel cycle where in the major actinides are recycled. The most preferred method for this task is solvent extraction, where in tri-*n*-butyl phosphate (TBP) is used as an extractant for more than seven decades.[1]In this context, the development of new molecules (ligands) for actinide separation and recovery is an active field of research. The development of ligands finds its application in the removal of actinides from lean solutions, separation of actinides and lanthanides, and development of better ligands for fast reactor fuel reprocessing, etc. Experimental studies in the past were dedicated to synthesizing and studying a large number of molecules for various applications. On the other hand, understanding the behavior of actinide extraction from a theoretical point of view and insights derived over time will help us tailor making an extractant for a specific application. In this regard, quantum chemical calculations are carried out to understand the complexation behavior of various ligands,[2] understanding the electronic structure and bonding,[3] and establishing the relationship between the ligand geometries and their properties.[4]The talk will focus on the development and application of density functional theory methodologies in the context of research work carried out at IGCAR, Kalpakkam.

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ST-09

Elemental Solids under High Pressure: A Case Study on Elemental Calcium

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Elements are the most fundamental materials and their behavior under varying thermodynamic conditions of temperature, pressure and volume has enormous importance in different branches of science. It has been observed that non-molecular elements mostly crystallize in the close-packed cubic and hexagonal structures at ambient conditions; however, startling complexities were observed in their high-pressure phase diagram. In some cases, elements adopt a non-periodic incommensurate/host-guest structure at high-pressure conditions. For example; barium metal (Ba) adopts a highly complex host-guest type structure which contains more than 700 atoms in the unit cell near to 12 GPa. In some other cases the elemental solids show spectacular changes in their physical properties at high-pressure conditions, for example, simple metals such as Li, Na, K, Mg, Cs turn into a semi-metal or an insulator when subjected to the extreme high-pressure conditions. It is widely believed that these elements form electrides under favorable high-pressure conditions, a novel class of materials containing localized electrons at the non-nuclear sites, i.e., at interstitial sites which acts like an anion. The electride in elemental solids at ambient or low pressure conditions are very rare though it is known for several organic and inorganic compounds. Presence of localized interstitial anionic electrons makes these solids suitable for many technological applications such as electron emitters, catalysts, battery anodes, optics, superconductors, etc.

Elemental calcium (Ca), a simple metal at ambient conditions, shows unusual high-pressure behavior in structural, electrical, and melting properties whose origin remain unsolved. Here, using a theoretical framework appropriate for describing electride phase formation, we establish electride formation in Ca at a pressure as low as 8 GPa which is analogue to a pseudo-binary NaCl (B1) type solid. For further compression we found Ca will directly transform from this FCC-electride phase to an SC-electride phase near 30 GPa which is analogue to a pseudo-binary CsCl (B2) type solid thereby avoiding the intermediate BCC phase observed in earlier experiments. By calculating pressure behavior of electrical resistance for the FCC-electride phase of Ca we shows that the pressure induced localization of the valence electrons at interstitial sites and expression of its anionic character is responsible for its strange pressure behavior. These findings are not limited to Ca but might hold a key to the understanding of host-guest type structures which occur in other elemental solids but at much higher pressure conditions.

ST-10

First Principle Tailoring of Metal Porphyrins for Electrocatalysis

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Porphyrins are a group of cyclic tetrapyrrolic compounds with four pyrrole subunits interconnected via methine bridges. The heterocyclic structure is a largely conjugated aromatic ring; that can in principle bind almost all metal ions to produce a four-coordinated structure. In nature, metalloporphyrins are involved in a wide variety of important biological processes, for example, hemoglobin and myoglobin. Metal porphyrins present an ample scope for tailor made application by modification of coordination environment of metal. This can be attained by addition of different types of ligands and modulation of electron and proton distribution by attaching acid/base groups on porphyrin group. The talk will highlight our density functional studies on Cobalt Porphyrin (CoPr) to design an efficient electrocatalyst for Oxygen reduction and evolution reactions (ORR/OER) that hold the potential as the means to provide sustainable energy solutions. Both reactions use precious metal-based electrocatalysts that are limited and expensive making a strong case to develop low-cost, active and stable electrocatalysts. Tailoring of CoPr framework by introducing meso phenyl substituents in the Pr ligand and further substitution of phenyl group by ortho/para-anilino groups yields an efficient and selective bifunctional catalyst that outperforms Ir/Ru and Pt based benchmark catalysts.

ST-11

Development of Artificially Intelligent Nanopores for High-Throughput Sequencing

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The potential for enhanced rapid sequencing methods could revolutionize preventive health care. Recently, solid-state nanopores have garnered significant attention for their promise in accelerated DNA sequencing. We have employed various artificial intelligence and machine learning tools to explore the sequencing of individual nucleotides [1-6]. In this presentation, we will provide a critical review of how machine learning tools are pivotal in the realm of third-generation DNA sequencing utilizing solid nanopore-embedded electrodes (**see Figure**).

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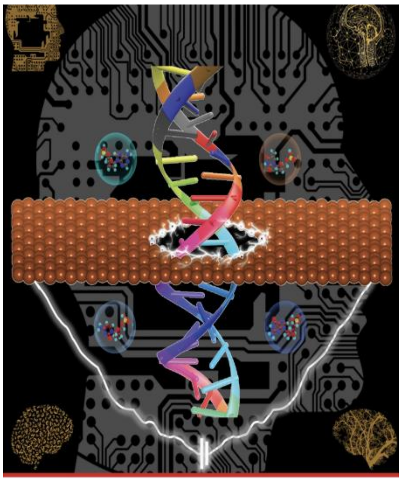

Figure: Solid State Nanopore for Rapid DNA Sequencing

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ST-12

Reinforcement Learning Helix Disrupting Mutation

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Helices are one of the most important secondary structural motifs within proteins. Often helix to random coil or helix to beta sheet transition leads to disruption of the protein and its function leading to numerous diseases. Although amino acids are categorized based on helix propensity scales that provide an idea about such helix disrupting mutations, the protein environment around the helix also dictates the stability of the helix. For a protein with n amino acids, there are ${}^{n}C_{k} \times 19^{k}$ possible k-point mutations possible. However, such a large number of trials are not practically feasible. Here, we employ reinforcement learning along with the state-of-the-art machine-learned protein structure prediction to tackle this challenge and develop a predictive model for helix-disrupting mutations. We start with a toy model consisting of helices with only 30 amino acids and train different models. Our results show that our model is successful in disrupting helical structures. We expand our methodology to effectively disrupt helices in proteins and confirm these outcomes through all-atom explicit water free energy calculations using well-tempered metadynamics. The results from our investigations serves as a proof-of-concept for developing similar models, showcasing the potential of reinforcement learning to tackle issues related to protein structure disruption.

Lightning Talks

LT-1

Exploring Boron Group Nanoclusters for Catalytic Activity

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Efficient catalysts play a significant role in advancing chemical transformations essential for energy conversion and storage technologies. This study introduces an integrated protocol that combines structure generation, property calculation using Conceptual Density Functional Theory (cDFT), and candidate selection to identify high-performance nanoalloys. Focusing on Group 13 elements (Boron, Aluminum, Gallium), we evaluated the oxygen reduction reaction (ORR) activity of these nanoclusters against platinum-based catalysts. Our approach provides a framework for identifying catalysts with comparable or superior catalytic properties, paving the way for the development of next-generation materials for sustainable energy applications.

LT-2

Relativistic Coupled Cluster Method Beyond Diatomic Molecules

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Modern chemistry addresses a variety of catalytic reactions involving different types of complexes and molecules. The diversity in bonding and the size of these species can make their simulation challenging. Furthermore, relativistic effects in larger or more substantial system (systems containing heavy elements) add to the computational complexity required for accurate simulations. The Relativistic four or two-component coupled cluster approach is the method of preference for accurate electronic structure calculations, because of the well-balanced incorporation of electron correlation effects as well as relativistic effects. However, the computational demands of the relativistic coupled cluster method limit its applications to small systems only, especially diatomic molecules. As a consequence, it is crucial to lower the computational cost of relativistic coupled cluster calculations in order to broaden their scope of usefulness. To lower computational costs, relativistic two-component methods have been developed, with the exact two-component (X2C) approach emerging as the most promising. Within X2C theory, the atomic mean field variant (X2C-AMF) is one of the powerful tool to improve the computational efficiency without a significant loss of accuracy [1]. The computational burden involved in relativistic two-component X2C-AMF calculations can be further lowered with the use of Cholesky decomposition scheme so that the construction of two-electron integrals and intermediates involving three and four virtual indices can be avoided [2]. Although the CD based X2C-AMF-CC implementations significantly lowers the memory and disc needs, the floating-point operation counts are comparable to those of the conventional implementations. To decrease the floating-point computations, one can use the natural spinors [3] which offers a compact representation of the correlation space and hence can further extend the applicability of CD based X2C-AMF-CC methods.

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LT-3

Relativistic Coupled-Cluster Study of Molecules for Precision Experiments

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Precision experiments with ultracold molecules are important for probing fundamental physics. Detecting *CP* violation (where *C* and *P* stand for charge conjugation and parity invariance, respectively), in particular, is crucial for exploring physics beyond the standard model. Here, we present four-component relativistic coupled-cluster calculations of several laser-coolable diatomic molecules to predict the *CP*-odd molecular sensitivity parameters necessary for analysing the results of precision experiments. Our study not only identifies suitable molecular candidates for such experiments but also provides precise sensitivity parameters of the molecules for interpreting the experimental results.

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LT-4

Electrode/Electrolyte-Based Interface Models for CO_2 Catalysis: A First Principle Study

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A heterogeneous catalytic environment (i.e., electrode/electrolyte) plays a major role to decide the catalytic activation and conversion of the CO_2 molecule at the interface.[1,2] In this work, we have performed first-principle calculations to study the adsorption mechanism of CO_2 at the interface. To examine this, the functionalized ionic liquid (IL) decorated Au(111) surface were selected for this, we have chosen functionalized 1-ethyl-3-methylimidazolium cation (i.e., $[EMIm\text{-}Z]^+[X]^-$; Where, Z = NH_2 and CF_3) with two different anions (i.e. $[X]^-$ = $[DCA]^-$ and $[SCN]^-$). To study the effect of functional groups in the alkyl chain, we have selected both electron-donating (i.e. $–NH_2$) and electron-withdrawing (i.e., $–CF_3$) groups with two different anions. Our results reveal that the electron donating groups ILs@Au(111) surface effectively activate and convert CO_2 to radical anion. But the electron-withdrawing (i.e., $–CF_3$) substituent lowers the binding strength of CO_2 and it slightly affects the electronic structure of the CO_2 molecule. Besides, the adsorption and activation mechanism of CO_2 at the interface is directly influenced by the involvement of the $-NH_2$ functional groups in the ($[EMIm]^+$) cation. In addition, the shift in the vibrational frequency confirms that the activation of CO_2 is occurred due to the introduction of functional group in ILs. Our work provides a guideline to the design and development of the functional materials for the selective carbon capture, activation, and conversion of CO_2 into other value-added products.[3]

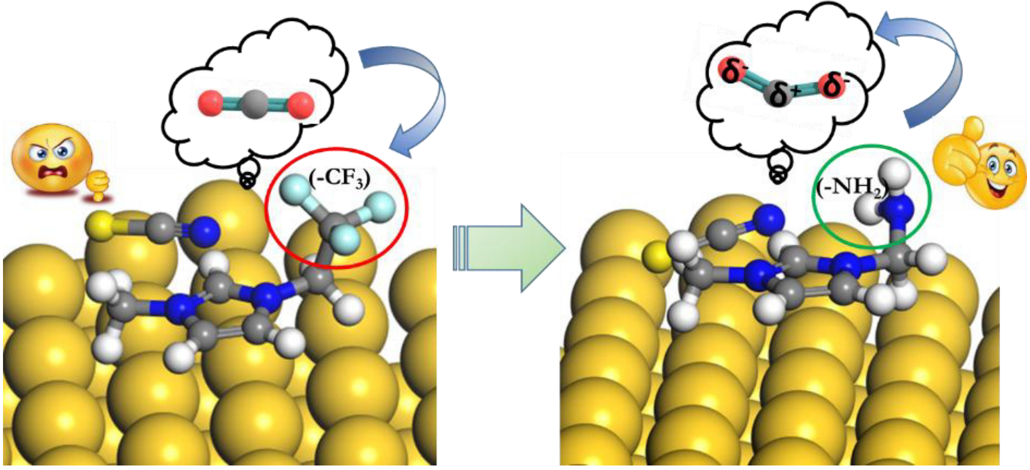

Figure 1. Electrode-Electrolyte Interface Models (IL@Au(111) Surface) for CO_2 Reduction Reaction

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LT-5

Computational Modeling of Materials for Energy Applications

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The power generation from conventional fossil fuels should be reduced due to its impact on global warming. In this context, energy production using nuclear energy and solar energy are promoted worldwide. Uranium dioxide (UO_2) is the predominant fuel in nuclear reactors for power production worldwide. During the nuclear fission of UO_2 fuel, many fission products are generated which are trapped in the fuel matrix. These fission products can amend the mechanical and thermo-physical properties of UO_2 fuel, which are a prime concern for nuclear safety. In this regard, we investigate the effect of different lanthanide (Ln) fission products on structural, mechanical, electronic and thermal properties of UO_2 [1,2,3,4]. The density functional theory (DFT) calculations employed here is improved for strongly correlated *5f* electrons of uranium using Hubbard-U corrections. The properties obtained from our *first principle* calculations show a good agreement with the available experimental and theoretical values. Metal clusters adsorbed on solid surfaces display size-dependent optical properties relevant to photovoltaics and to photocatalysis. In this work, we deal with the theoretical and computational modeling of the photophysics of rutile TiO_2(110) surface with and without adsorbed silver clusters. The presence of Ag adsorbates creates new electronic energy levels in the energy band gap region of the substrate TiO_2 slab, which are relevant to photoexcitation. The photoexcitation of electrons from valence to conduction band lead to electron transfer from the adsorbates to the slab and to substantial increases in the absorption flux of light in the near infrared, visible and near ultra-violet regions of the spectrum [5]. In another study, we investigate the optical properties of crystalline silicon slabs and their nanostructured surfaces without and with adsorbed silver (Ag) clusters. Results on light absorption are quite different for the two DFT functionals (PBE and HSE06), and are presented here for light absorbances using orbitals and energies from the hybrid functional giving correct energy band gaps. The calculated range of absorption energies overlaps with the range of solar photon energies, making the present structures and properties relevant to applications to solar photoabsorption and photocatalysis [6].

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LT-6

SUB-PICO-NEWTON FORCES AND THE FOLDING-UNFOLDING OF TRPZIP2 Β-HAIRPIN

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Folding-Refolding of proteins are often affected by various factors [1], which include a significant contribution from the solvent environments and the subtle mechanical forces they impart. For example, the thermal motion of the solvent could readily impart few tens of piconewtons of force on the protein. [2] Further, living cells are subjected to mechanical tensions owing to pressure gradients and mechanical translocations. The structural aberrations caused by these forces can directly affect the folding-unfolding mechanism of the proteins inside the living systems. TrpZip2, a 12-residue model β-Hairpin protein, is schematized here to assess the folding-unfolding process under the influence of a mechanical bias.

The effect of forces on the protein folding-unfolding was studied using metadynamics simulation under no external force and with an external bias. 30 pN force was chosen such that the protein does experience a net effective force, yet preserving the morphology of TrpZip2. We found that in both null external force and 30 pN bias, TrpZip2 exhibited a zip-out mechanism for folding-unfolding, but the folding pathways in both scenarios were distinctive. The hairpin turn showed high stability in the presence and absence of external force, thereby initiating the folding process. Most importantly, the cause of the diverse behavior of TrpZip2 towards folding-unfolding was found to be the existence of wide conformations that can be achieved via different trapped intermediates while experiencing irregular forces surrounding them. [3]

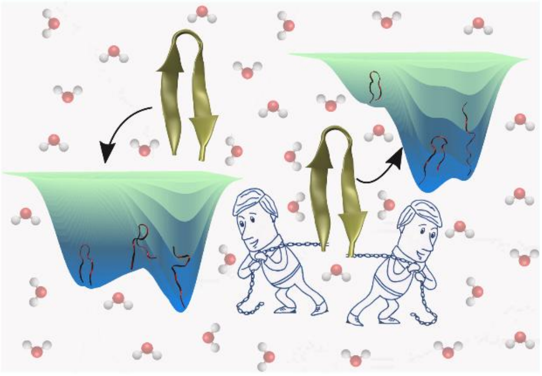

Figure 1. Different folding pathways of TrpZip2 hairpin with no external bias and 30 pN external bias.

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LT-7

Accelerating Materials Discovery for Catalysis and Electrochemical Energy Storage

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The rapid discovery of advanced materials with superior performance through large-scale computational screening is crucial for the development of future technologies in energy conversion and storage. Inverse materials discovery, which leverages electronic structure to design materials with specific properties, offers a powerful and cost-effective approach to expedite this process. This methodology not only guides experimental efforts toward the most promising material candidates but also optimizes the use of human resources and efforts. In this presentation, I will introduce an inverse materials discovery methodology and present a computational strategy to accelerate rational materials discovery. This strategy combines First-Principles Density Functional Theory calculations with Machine Learning interatomic potentials (MLIPs) to design stable and efficient cathode materials for high-capacity Sodium-Ion Batteries (SIBs) and to elucidate electronic structure-activity relationships for key catalytic reactions. Furthermore, I will demonstrate the capability of Machine Learning interatomic potentials to accurately pre-screen a wide range of crystal structures for applications in catalysis and electrochemical energy storage.

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Figure: Schematic representation of accelerated discovery approach.

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LT-8

Tuning Intrinsic Defects through Dopant Engineering

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Engineering defects in materials constitutes a key approach to control several important properties including electronic, optical, magnetic, and catalytic properties for various industrial and technological applications. Moreover, as a result of thermal equilibrium and the kinetics of processing, all real materials contain structural defects which could significantly affect their properties. Here, I will mainly discuss my research activities on designing of tunable materials through dopant and defect manipulation for clean energy applications and optoelectronics devices.[1,2]

Wide band gap semiconductors with high dielectric constant and good thermal dissipation are very popular for wide range of optical and electronic devices. In the recent studies $ZnGa_2O_4$ has been projected as an alternative to Ga_2O_3. The structural simplicity (face-centered-cubic spinel structure) results into isotropic electronic and optical properties for $ZnGa_2O_4$, in comparison to the large anisotropic properties for the β-monoclinic variety of Ga_2O_3. Recent experimental observation indicates that the doping with Ge into $ZnGa_2O_4$ improves the optical properties. However, an unambiguous and ultimate explanation on microscopic origin of the experimentally observed optical property and the limiting factors has not been accomplished so far. This drives us to gain a detailed knowledge of the defect chemistry in Ge-doped $ZnGa_2O_4$. Present study nicely explains the experimental observation of colour variation property of $ZnGa_2O_4$ by oxidation-reduction process. The experimental observation of poor optical behavior in the presence of oxygen vacancy and improvement due to doping with Ge have been explained. Present study showed that the presence of Ge favors formation of gallium vacancy, which can reduce the band gap significantly without the involvement of discrete midgap trap states, resulting into enhanced optical output. This unique strategy can be applied to large number of materials for the enhancement of their optical properties.

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LT-9

Modeling, Theory, and Simulation in Soft Condensed Matter (F) Nature of universal subdiffusion crossover in molecular glass-formers

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The issue of diffusion in supercooled liquids and glasses is a key element in understanding glass transitions. These materials don't follow typical Brownian motion principles, such as linear time-dependent mean-squared displacement and Gaussian displacement distribution. The deviations from these features depend on the scales considered and lead to shifts between different diffusion mechanisms. Universally, molecular/polymeric glass formers exhibit a crossover from non-Gaussian to Gaussian subdiffusion [1-2]. Despite extensive simulation and experimental work on this universality, a fundamental model hasn't been established, preventing a comprehensive picture of the underlying non-Gaussian behavior. In particular, the universal exponential tails observed as a signature in van Hove self-correlation of glassy relaxation has not been established in these non-Gaussian subdiffusive phenomena. In this work, we develop a model based on non-Gaussian fractional Brownian motion (nGfBm), extending the fBm model to incorporate non-Guassian features using a jump-kernel [2]. Employing the Fokker-Planck equation for this model, we describe the subdiffusion crossover as observed using incoherent quasielastic neutron scattering (IQENS). It is notable that the non-Gaussianity in the subdiffusion process is fundamentally driven by an exponential jump-kernel which is governed by a characteristic jump length and waiting time. By obtaining the exact solutions for the case of exponential jump-kernels, we calculated van-Hove self-correlation functions in the strongly non-Gaussian limit, as shown in Fig. 1 for pure ethylene glycol. The exponential tails in the van Hove self-correlation function are clearly evident in the non-Gaussian limit of the relaxation which is observed for $t < 20$ ps, typically waiting times in the system.

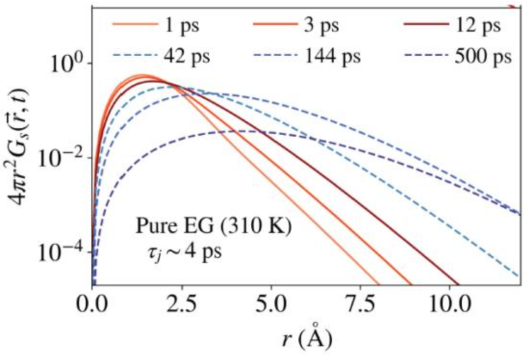

Figure 1: The radial van Hove self-correlation function calculated based on IQENS measurements on ethylene glycol (EG) at 310 K. Here τj is the characteristic waiting time between jumps in the diffusion process.

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Contributory Papers

Category A: Recent Advances in the Theoretical Formalisms and Simulation Methodologies

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Category C: Modeling, Theory, and Simulation in Nuclear Waste Management Research

Category D: Computational Chemistry Related to New Generation Nuclear Fuels

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Category I: Experiment Driven Theoretical Investigations

Category J: Modeling, Theory and Simulation for the Exploration of Biological Phenomena and Drug Design

A-122

Enhanced Sampling Approaches to Study the Self-Assembly of Calcium Cholate in Aqueous Media

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Low molecular weight gels (LMWG) have been of tremendous interest in the supramolecular community due to their utility in tissue engineering, sensors, light emitting materials, drug delivery systems, etc. Herein, we computationally study the self-assembly behaviour of calcium cholate (CaCh, Figure 1) in water. Experimentalists reported [1] that CaCh forms spherical aggregates of diameter 100-150nm (Figure 2a) which transforms into a self-supporting gel in three hours. The spherical aggregates join to form the gel network, with each fiber of height 6-10 nm (Figure 2b), as measured with AFM.

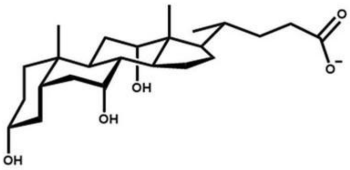

Figure 1: single cholate anion

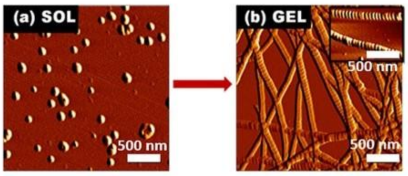

Figure 2: AFM image of CaCh in (a) spherical aggregate, (b) gel

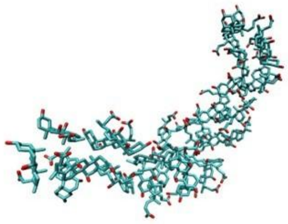

Figure 3: cholate fiber in water

Molecular simulations on self-assembled, one-dimensional aggregates which offer a quantitative comparison to experimental results as in the current case are nearly absent in the computational literature. Our initial all-atom molecular dynamics (MD) simulations for a small system size carried out in explicit solvent revealed signatures of a fibrous arrangement of CaCh (Figure 3). The diameter of the fibers observed in simulations is nearly half of that reported experimentally. An extensive analysis demands a bigger system size, but the increase in simulation time imposes significant constraints. It motivated us to employ enhanced sampling methods such as REST2 [3] and REHT [4] which have been widely used for studying biomolecular systems, but not for self-assembly. However, despite optimizing various parameters, these techniques prove to be of limited effectiveness. Results from these approaches will be presented in detail. Currently, alternative approaches like CVHD [5] and enthalpy mediated strategies [6], are being explored.

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A-123

Effect of Metal Based Anion in Ionic Liquid@UiO-66 MOF for Selective CO_2 Capture and Separation: A Computational Study

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The carbon capture from flue gases is an important step to fight global warming and climate issues due to the fact that CO_2 is consider to be a main cause for global warming [1]. In past decade researches were carried out to identify a potential candidate for CO_2 capture and separation from the flue gas. Ionic Liquids (ILs) and metal organic framework (MOF) are two well-known materials in the field of CO_2 capture [2,3].In this work we have selected UiO-66, a Zirconium based MOF with several ILs which has common cation as $[EMIM]^+$ and various anions such as $[Cl]^-$, $[AlCl_4]^-$ and $[FeCl_4]^-$.To understand the effect of metal based anion in CO_2 capture and it's selectivity over other gases,selected ILs were impregnated in *Octahedral* (*Oh*) and *Tetrahedral* (*Td*) pores of UiO-66 [3]. It is found from calculations that the selectivity of CO_2 increases with increase in spatial confinement. Heat of adsorption of CO_2 is relatively higher for $[EMIM]^+[AlCl_4]^-$ @ UiO-66 composite. Selectivity of CO_2/CH_4 and CO_2/N_2 was evaluated for selected ILs@UiO-66 composites.Our study will depict a molecular level understanding towards effective CO_2 capture and its separation.

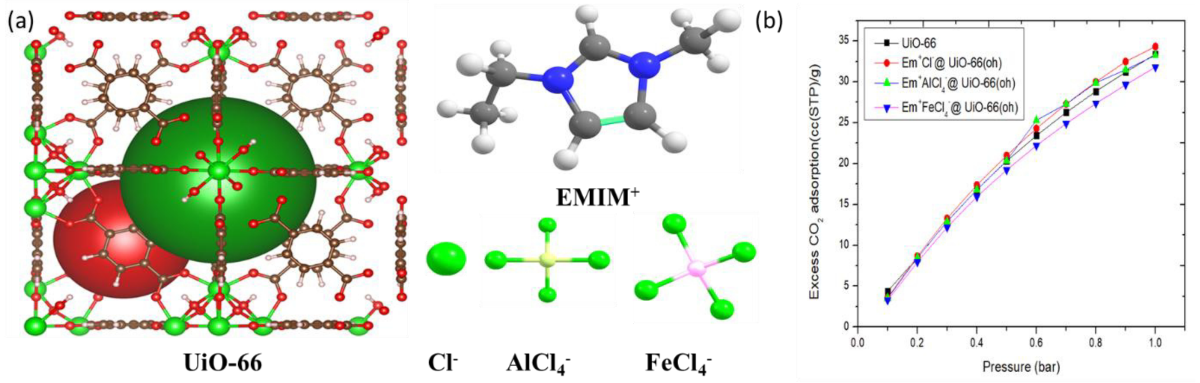

Figure 1. (a) UiO-66 with two different pores and Selected ILs, (b) Single adsorption isotherm of CO_2 on selected materials**.**

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A-124

Application of Parametric Equation of Motion to Precise Identification of LUMO

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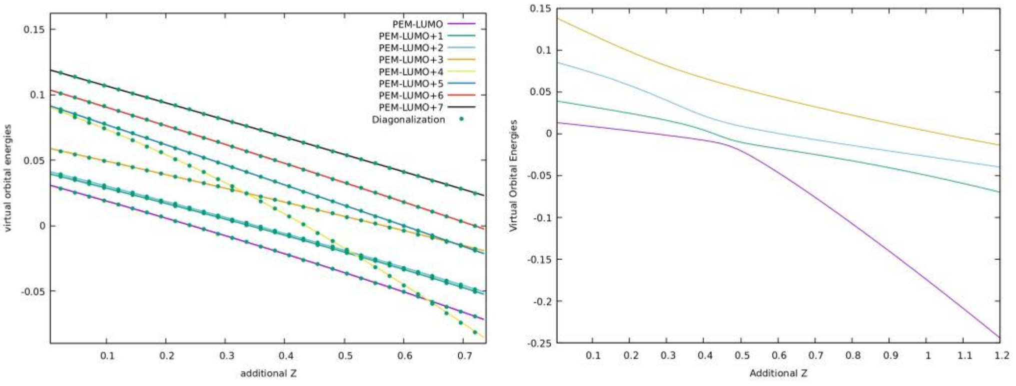
The lowest unoccupied molecular orbital (LUMO) plays a crucial role in quantum chemistry. However, existing quantum chemistry calculations struggle to provide useful virtual orbitals, which complicates the study of various processes such as photochemical reactions, electron attachment, reduction, and excitation. Identifying the LUMO obtained from the self-consistent field (SCF) solution is crucial, as it frequently exists among states with nearly similar energies. The nuclear charge stabilization method has proven valuable in identifying the LUMO. The application of parametric equations of motion (PEM) in conjunction with the nuclear charge stabilization method is proposed to accurately identify the LUMO from the SCF solution [1]. Nonetheless, incorporating additional diffuse functions into the basis set, essential for characterizing electron-attached and electron-excited states, can introduce complications due to the presence of states with identical symmetry, leading to avoided crossings. Identifying the true LUMO amidst these avoided crossings becomes challenging due to the mixing of states and the exchange of their orbital character. Modification of the PEM [2] is implemented to accurately pinpoint the true LUMO by preventing the stabilization of specific states involved in avoided crossings, proving to be a highly effective approach with minimal computational cost.



(a) (b)

Figure 1. Charge stabilization plot for neutral C_2H_4 molecule a) using aug-cc-pVTZ basis set b) using cc-pVDZ+5p basis set .

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A-125

Hydrogen Doping in Metal Nanoclusters: A DFT Study on Reducing Activation Energy in CO Oxidation

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Mechanisms of chemical reactions are typically explored by identifying stationary points on the potential energy surface, which include both minima and saddle points. Minima represent the stable states such as reactants, products, and intermediates, while saddle points correspond to transition states that connect these minima. Essentially, the reaction pathway is traced by moving from one minimum (reactant or intermediate) to another through the transition state, which represents the highest energy point along the pathway.Carbon monoxide (CO) is a harmful pollutant produced by incomplete combustion in engines and industrial processes.The conversion of carbon monoxide (CO) is a critical process in various industrial applications, such as the synthesis of hydrocarbons and the reduction of CO emissions. Doping metal nanoclusters with other elements can significantly influence their catalytic performance by modifying the electronic structure, altering the adsorption energies of reactants, and stabilizing different transition states (TS). This study explored how doping metal nanoclusters affects CO oxidation by focusing on the activation energy and the role of the transition state in the reaction pathway. Weuse DFT to design and optimize catalysts that can efficiently convert CO to less harmful CO_2 .Density Functional Theory (DFT) has emerged as a powerful quantum chemical method to investigate the mechanisms underlying CO conversion, providing insights into the activation energy, transition states, and the role of CO in catalytic processes.

Here we report, how the Hydrogen dopant [1] influences the stabilization of the transition state and the overall activation energy. The dopants selected for this study included various coinage metals (Such as: Au), known for their ability to enhance catalytic activity through electronic and geometric effects. The presence of a dopant alters the charge distribution within the nanocluster, leading to changes in the adsorption energy of CO and other reactants. Doping not only modifies the electronic properties but also induces structural changes that stabilize the transition state, leading to more efficient CO conversion [2]. Furthermore, the analysis of the transition state revealed that the geometric configuration of the doped nanocluster plays a crucial role in determining the activation energy. The comparison between doped and undoped nanoclusters highlighted the importance of carefully selecting dopants to optimize the catalytic performance for specific reactions.These findings suggest that optimizing these catalysts can lead to more effective methods for reducing CO emissions, thereby mitigating their harmful environmental impact. Our results indicate that hydrogen doping metal nanoclusters can significantly lower the activation energy required for CO oxidation.

In summary, hydrogen doping of metal nanoclusters improves their catalytic efficiency in CO oxidation by lowering activation energy and stabilizing the transition state. Future research should investigate different dopants and conditions, validate these findings experimentally, and explore practical industrial applications for environmental protection.

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A-127

Relativistic Coupled Cluster Beyond Diatomic Molecules

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Recent advancements in chemistry focus on a variety of catalytic reactions that involve different types of complexes and molecules. The diversity in bonding and the size of these species can make their simulation challenging. Furthermore, relativistic effects in larger or more substantial system (systems containing heavy elements) add to the computational complexity required for accurate simulations. The Relativistic four or two-component coupled cluster approach is the method of preference for accurate electronic structure calculations, because of the well-balanced incorporation of electron correlation effects as well as relativistic effects. However, the computational demands of the relativistic coupled cluster method limit its applications to small systems only, especially diatomic molecules. As a consequence, it is crucial to lower the computational cost of relativistic coupled cluster calculations in order to broaden their scope of usefulness. To lower computational costs, relativistic two-component methods have been developed, with the exact two-component (X2C) approach emerging as the most promising. Within X2C theory, the atomic mean field variant (X2C-AMF) is one of the powerful tools to improve the computational efficiency without a significant loss of accuracy [1]. The computational burden involved in relativistic two-component X2C-AMF calculations can be further lowered with the use of Cholesky decomposition scheme so that the construction of two-electron integrals and intermediates involving three and four virtual indices can be avoided [2]. Although the CD based X2C-AMF-CC implementations significantly lowers the memory and disc needs, the floating-point operation counts are comparable to those of the conventional implementations. To decrease the floating-point computations, one can use the natural spinors which offers a compact representation of the correlation space and hence can further extend the applicability of CD based X2C-AMF-CC methods.

The goal of this work is to lift storage limitations and reduce the floating-point operations simultaneously that are involved in relativistic calculations and extend the approach's applicability to medium-sized molecules through the low-cost development of a two-component (X2C-AMF) coupled cluster (CC) and equation-of-motion coupled cluster (EOM-CC) method based on Cholesky decomposition (CD) and frozen natural spinors (FNS). The CD and FNS based X2C-AMF coupled cluster and equation of motion coupled cluster methods have been successfully implemented into the development version of our in-house software, BAGH (https://sites.google.com/iitb.ac.in/bagh/). To check the performance of the CD-FNS-CCSD and CD-FNS-CCSD(T) methods, we have chosen to calculate the gas phase non-covalent bond dissociation enthalpies of few coinage metal complexes. For the CD-EOM-CCSD method, ionization potential variant of EOM (IP-EOM-CCSD) is used and the performance was tested by calculating the vertical ionization energies of a test set containing heavy elements. From the results obtained, it was found that the enthalpy values were well within the experimental uncertainty for normal cutoff and for ionization energies it was loose cutoff, maintaining a balance between accuracy and computational efficiency. From the results, we can confirm that the present implementation can be extended to calculate non-covalent bond dissociation enthalpies and vertical ionization energies for medium-sized metal complexes where the four-component method becomes computationally expensive. The comparison of the computational timings of the two-component CD-FNS-EOM-CCSD with the corresponding four-component FNS-EOM-CCSD shows that the two-component CD-FNS-based relativistic calculations only take a fraction of the timing of the corresponding four-component variants suggesting the routine use of CD-FNS-CC/EOM-CC method in computations involving metal catalysis or complexes.

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A-128

Towards Efficient and Accurate Excited State Calculations: Combining lower scaling Approximations and Tensor hypercontraction

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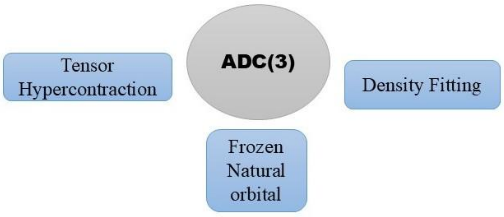
Time-dependent density functional theory (TD-DFT) is a widely used method for calculating excited state properties, similar to the configuration interaction singles (CIS) method, due to its reasonable computational cost for low-lying valence excited states. However, a significant drawback of TD-DFT[1] is the occurrence of spurious charge transfer states caused by the exchange-correlation functional. The wave function based methods are free from that problems. Among all the single reference wave function based methods are available in the literature[2], coupled cluster model like CCS(CIS), CC2, CCSD and more hierarchy method gives almost accuracy with increasing computational cost. In addition to coupled cluster methods, algebraic diagrammatic construction (ADC) methods like ADC(2), ADC(2)-x, and ADC(3) are also popular for calculating excitation energies. While CC2 and ADC(2) are lower scaling methods for vertical excitation energies, they fail for Rydberg-type states of molecules. Therefore, it is necessary to go beyond CC2 and ADC(2). However, methods like EOM-CCSD[3] and ADC(3)[4] have N^6 scaling, which limits their applicability to molecules with fewer than ten atoms. A lot of effort has already been devoted towards reducing the computational cost. All the lower scaling approximation to this higher method can be classified three distinct categories. The first category of method involves truncation of the wave function using localized and natural orbitals[5]. The second category method employs perturbation truncation of the ground and excited state wave functions to reduce the computational cost of these hierarchy methods. However, as any other perturbative approximations the accuracy of the methods depends upon the availability of suitable zeroth order reference state and does not provide uniform accuracy for all kinds of excited states. The third kind of approximation involves approximating the two electron integrals using density fitting[6] approximations. But it leads to reduction of scaling of coulomb type of integral not the exchange one. However, the scaling of exchange integrals can be reduced using tensor hypercontraction[7]. So, we can expect combining all these approximations reduces the scaling and gives accuracy for calculating all type of valence, charge-transfer and Rydberg excited states.



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A-129

Leveraging Natural Spinors for Precise and Efficient Estimation of Heavy Atom and Molecular Properties on Quantum Computers

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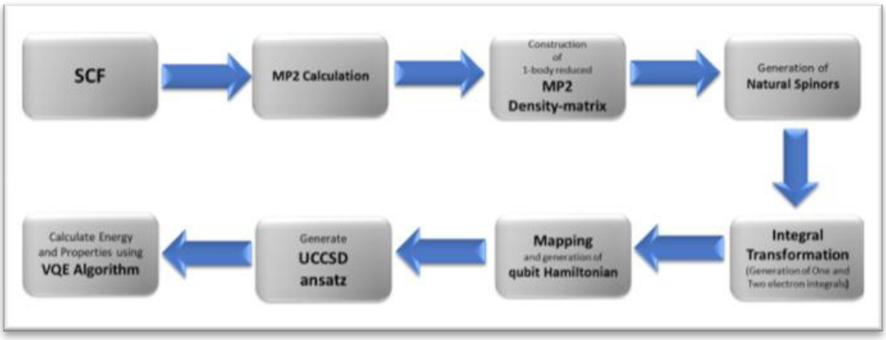
We present an efficient scheme to calculate atomic and molecular energies and properties for heavy atoms and molecules on quantum computers. Relativistic effects are vital for the accurate description of heavy elements, making the 4-component Dirac-Hartree-Fock (DHF) method a critical starting point. However, the computation of one-body and two-body integrals in DHF becomes a bottleneck for larger molecules. To overcome this barrier, we have used exact two-component atomic mean field (X2C-AMF)[1] instead of 4-component Dirac Hamiltonian.

The Variational Quantum Eigensolver(VQE)[2] is a widely recognized quantum-classical hybrid algorithm designed for Noisy Intermediate-Scale Quantum (NISQ) systems.Its applicability in relativistic quantum chemistry has been rigorously validated by Das and coworkers[3,4].The computational expense of VQE is heavily affected by the qubit-Hamiltonian size, which is constructed from the mapped one-body and two-body integrals generated via SCF calculations.We have employed an effective active space framework that reduces the size of the virtual space through classical preprocessing using natural spinors.The naturalspinors are derived through the diagonalization of the one-body reduced density matrix formed with the help of the MP2 wavefunction.[5] The efficacy of natural spinors/orbitals is well-established in conventional classical quantum chemistry. Recent studies by Zaribafiyan and coworkers[6] demonstrate that natural orbitals can be equally effective in for non-relativistic VQE calculations. In this work, we showed that natural spinors can greatly reduce the computing cost of relativistic VQE calculations. Moreover, the use of perturbative corrections further improves the results.



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B-122

Development of a Machine Learning Potential for Glassy B_2O_3 Under High Pressure

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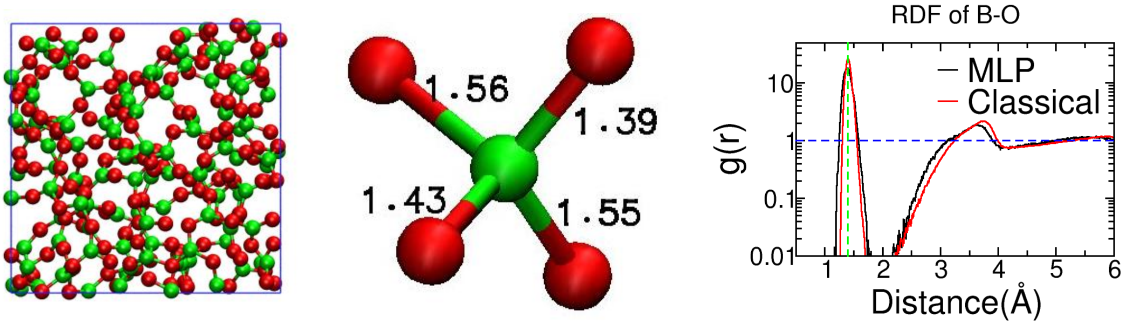
Atomistic simulations of B_2O_3 and alkali borosilicate are challenging partly because of the varied coordination environments of B and O, especially at high pressures[1]. Traditional empirical force field based molecular dynamics simulations show starkly contrasting trends in the interatomic structure based on their parameters. On the other hand, First-Principles Molecular Dynamics (FPMD) simulations can capture the coordination well at various temperature and pressure ranges but are computationally expensive[2]. Here, we developed a Machine Learning Potential (MLP). based on Density Functional Theory calculations, to understand the short- and intermediate-range order in B_2O_3 over a wide range of temperature (300-3000K) and pressure (0-200GPa). The MLP based simulations is as accurate as FPMD at a fraction of the computational cost of the latter. The evolution of boron coordination number, medium range order, ring structures, and the structure factor of glassy B_2O_3 under these conditions have been examined. In Figure 1, (a) shows one snapshot of glassy B_2O_3 (b) one 4-coordinated Boron atom with oxygen and (c) shows the RDF of B-O compared with the classical Force Field. the first peak value of RDFs is collected in Table 1 for both MLP and Classical Force Fields.



(a) (b) (c)

Figure 1. (a) Snapshot of glassy B_2O_3 modelled with MLP (b) Illustrative four coordinated B-atom connected to oxygens. (c) Radial distribution functions of B-O obtained with MLP and using an empirical force field[1].

Table 1. Comparison of key interatomic distances

RDF	MLP (Å)	Classical Force Field (Å)
B-O	1.38	1.39
B-B	2.56	2.72
O-O	2.41	2.41

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B-123

A Machine Learning Approach to Decipher the Origin of Magnetic Anisotropy in Three-Coordinate Cobalt Single-Ion Magnets

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Single Molecule Magnets (SMMs) are essential as models for permanent magnets and play a key role in compact information storage and molecular spintronics. The magnetic anisotropy, particularly the axial zero-field splitting parameter (D) in mononuclear transition metal complexes, is crucial in determining SMM behavior.[1] Low-coordinate mononuclear transition metal complexes, in particular, exhibit significant anisotropy and higher blocking temperatures compared to other molecular classes. However, predicting the sign and magnitude of the D value is a complex task influenced by donor atom characteristics and structural parameters. [2]

To tackle this challenge, an initial dataset of 90 Co (II) complexes was carefully curated and later expanded to 614 complexes through optimization techniques. Predictions of D values and their sign classification were attempted, but traditional magneto-structural correlations fell short in explaining observed trends. To overcome this, machine learning tools were employed, identifying seven key descriptors that influence D values: bond lengths (BL1, BL2, BL3), bond angles (BA1, BA2, BA3), and the parameter ϕ. These descriptors were used to construct a dataset of 614 complexes, which was then randomly shuffled and split, with 80% used to train the model and 20% to test its predictive capabilities. Our model achieved over 90% accuracy in test predictions and over 95% accuracy in classification, as demonstrated in Figures 1(a) and 1(b). This approach aimed to uncover the complex relationship between structural features and magnetic properties, advancing the understanding of SMM behavior in mononuclear transition metal complexes.

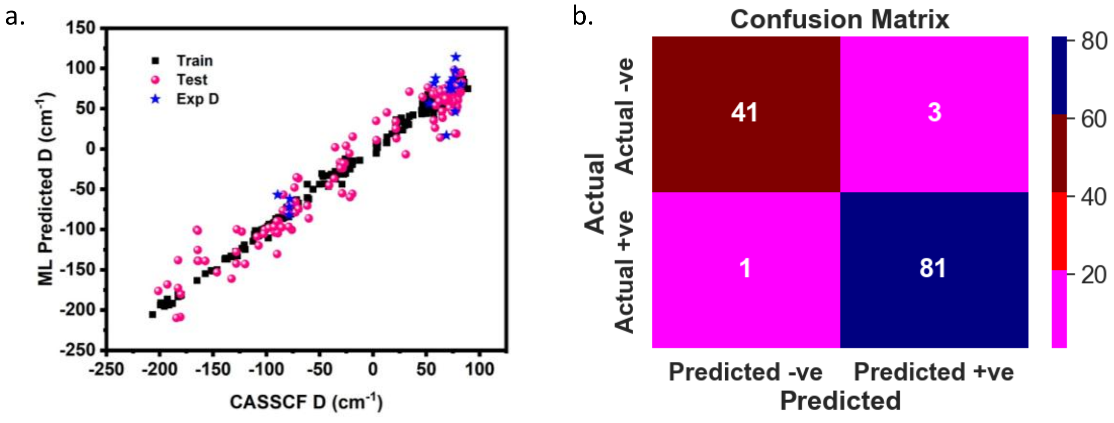

Figure 1. (a) Scatter plots illustrate the comparison between ML-predicted, CASSCF-calculated D, and experimentally reported values within both training and testing data sets. (b) Binary confusion matrix with an actual sign on the y-axis and predicted sign on the x-axis.

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B-124

How do quantum chemical descriptors shape hydrogen atom abstraction reactivity in cupric-superoxo species? A combined DFT and machine learning perspective

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Oxygen activation, a crucial function performed by enzymes, prompts the synthesis of biomimetic models utilized to investigate structure–activity relationships, with a particular focus on metal-superoxo species resulting from O_2 interaction with the metal center. Among others, cupric-superoxo species have been extensively studied, showcasing diverse examples and potent catalytic capabilities. While quantum chemical calculations have helped in understanding the mechanistic aspect of their reactivity, recent advances in machine learning (ML) tools have substantiated this further and offered potent predictive power. The development of machine learning tools and associated quantum descriptors for open-shell paramagnetic catalysts is rarely pursued due to the complexity involved. However, if achieved, it has the potential to fundamentally change the existing paradigm in catalytic design and development. In making this connection, a detailed hydrogen atom transfer (HAT) reaction instigated by $[(\text{TMPA})\text{Cu(II)}–O_2^{\cdot -}]$ (TMPA = tris(2-pyridyl methyl)amine) (Figure1) species and its analogues gains relevance as they offer a unique set of diverse reactivity pathways among structurally similar cupric-superoxo species. In this study, we embark on a comprehensive exploration of reactivity mechanisms employing the DFT method (B3LYP/TZVP) with five distinct catalysts and three varied substrates, resulting in combinations that lead to fifteen different reactions for the HAT reaction. [1] The reactivity of cupric-superoxo species was found to be correlated not only with the rate-limiting HAT barrier but also with the competitive dimerization barrier. Our comprehensive analysis of mechanisms offered a rationale for the experimentally observed reactivity and the setting of goals for developing suitable ML models. In making this connection, we have arrived at fifteen quantum chemical descriptors, including exchange interaction (J), sterics, hydrogen bonding, and various thermodynamic parameters derived from DFT calculations. Our multivariate linear regression (MLR) model accurately predicts catalytic reactivity towards HAT using these quantum chemical descriptors based simply on ground state geometry. The H-bonding interactions, along with the free energy of the HAT/PT/ET reaction ($\Delta G_{\text{PCET}}/\Delta G_{\text{PT}}/\Delta G_{\text{ET}}$), were found to yield excellent results for accuracy ($R^2 = 0.90$), setting a stage to study multinuclear paramagnetic catalysts. For the first time, this study provides valuable insights not only into the reactivity of metalloenzymes but also offers design clues to enhance the reactivity of transient species using the ML approach.

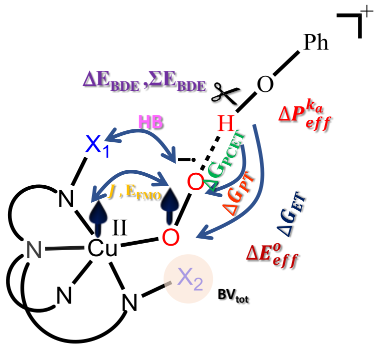

Figure 1. Schematic representation of encoding the catalyst structure and various quantum chemical descriptors employed

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B-125

Property Guided Inorganic Molecule Generation

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Functional Materials with tailored properties are essential for advancements in energy storage and semiconductors. Despite the advancements in generative models, producing materials for specific purposes remains challenging. In this study we introduce an approach to the generative design of inorganic materials, employing a string-based, invertible representation called Simplified Line-Input Crystal Encoding System (SLICES) [1]. This representation adheres to crystallographic invariances, facilitating accurate modelling and the reversible generation of crystal structures. Our research specifically addresses the complex challenges of single and multi-objective inverse design of crystals, enabling the creation of de-novo crystal structures with precisely tailored properties. We integrate a transformer decoder model with a unique property-guided generation mechanism.

By introducing special tokens corresponding to specific material properties such as bulk modulus, band gap and formation energy, we create a unique control mechanism for material generation. The embedding of these special tokens is scaled using the desired property values, allowing for fine-grained control over the generated structures.Furthermore, by facilitating multi-objective design, our approach goes beyond single-property optimization. The result shows our generative model's capability for precise material design. In particular, our ability to produce materials with exact composition, electrical properties, and mechanical properties marks a significant advancement toward creating more robust next-generation materials. The framework for property-guided inorganic molecule generation proposed in this study can potentially transform the field of material discovery and development.

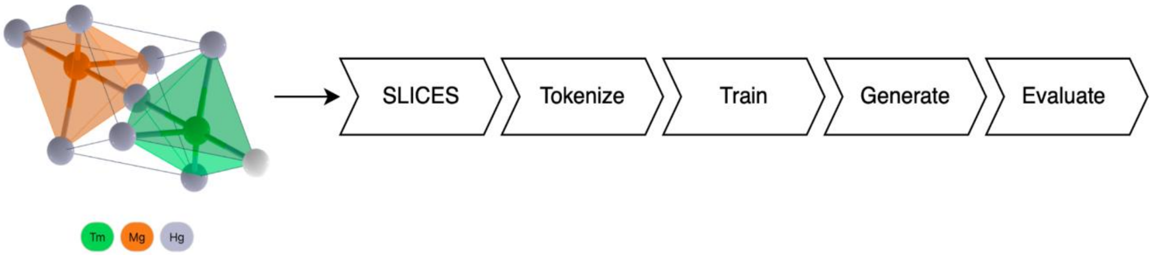

Figure 1. Depiction of the workflow of the work reported here

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B-127

Integration of Density Functional Theory and Machine Learning for Electrolyte Optimization in High-Voltage Dual-Ion Battery Design

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Designing DIBs by using various electrolytes through experiments or computationally is highly time consuming and needs high-cost sophisticated resources. Here, we have utilized ultrafast screening capability of machine learning (ML) for searching suitable salt-electrolytes towards designing of DIBs, choosing voltage as the desirable descriptor. Considering 50 different salts and their suitable staging mechanisms (Figure 1), XGBoost Regressor ML model has been found to perform with remarkable accuracy. This is further validated by density functional theory, cross-validation, and experimental findings. An interpretable ML technique, SHapley Additive exPlanations (SHAP) analysis has been employed for local and global feature analysis to interpret the ML predicted result, underscoring the importance of choosing input features. Staging mechanism, number of intercalated anions, oxidation state of cations, and formula weight of anions emerged as critical features influencing voltage prediction as identified by SHAP analysis. Monovalent cations like Li, Na, and K are found to deliver higher voltages compared to divalent cations like Mg and Ca. This ML assisted DIB design approach has the potential to explore unknown salt-electrolytes that are yet to be tested in DIBs. Finally, we introduce the predicted voltages for all the salt-electrolyte combinations as well as their probable staging mechanism. We signify the absence of a general trend in the predicted voltages as various combinations of cations and anions are found to deliver unique voltages. Our study can guide researchers towards tuning constituent salts as well as staging mechanisms for the design of efficient DIBs.

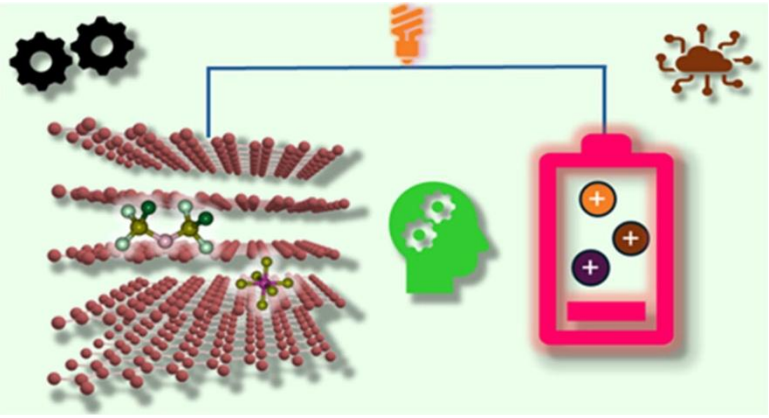

Figure 1. Machine learning based prediction of voltage for various electrolytes considering graphite as cathode.

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B-128

Improving Yield Prediction in Cross-Coupling Reactions Using a Regression Transformer Model with Augmented SMILES Data

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Accurate prediction of yields in cross-coupling reactions is vital for optimizing chemical synthesis processes. In this study, we explore the use of a Regression Transformer model to predict yields of cross-coupling reactions. The Regression Transformer model achieved an R^2 value of 0.24, reflecting difficulties in capturing the complex relationships among reactants, catalysts, and products. To address this, we employed data augmentation techniques, such as randomization and permutation, to expand and diversify the dataset. This enriched dataset provided the model with a broader range of training examples, enhancing its ability to learn from diverse chemical scenarios. After retraining the modified model on this augmented data, we observed a significant improvement in predictive performance, with the R^2 value increasing to 0.57. This notable enhancement underscores the efficacy of integrating data augmentation with a Regression Transformer model. Our approach demonstrates that a well-tuned Transformer model, coupled with comprehensive data augmentation, can substantially improve yield prediction accuracy in chemical reactions. This advancement offers valuable insights for optimizing chemical processes, leading to more efficient and accurate outcomes.

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B-129

New Developments and Applications of Graph Neural Network Approach for Accelerated Cluster Structure Prediction

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Theoretical prediction of energetically stable cluster or crystal structures from their constituents is a significant problem, with substantial applications in material science [1-5].We present a graph neural networkapproach(GNN) for predicting stable nanocluster structures on their potential energy surfaces (PESs). GNN-based model assists in the structure building of atomic metal clusters with specific sizes and point-group symmetry. This approach is benchmarked on the prototype Mg_nclusters with $n < 150$. Moreover, the ground state structures of Mg_n $(n = 4\text{-}32)$ clusters generated through GNN approach corroborate well with the global minimum structures reported in the literature. Further, this approach could generate novel symmetric isomers of medium to large Mg_nclusters in the size regime, $n < 150$, by constraining the point-group symmetry of the parent clusters. The *growth potential* (GP) of a cluster gives a measure of its parent cluster to accommodate more atoms and characterize the structures on the GNN-guided path. Along the highest GP paths, GNN approach is further employed to generate stable Mg_n nanoclusters with $n = 228, 236, 257$ and 260. Therefore, GNN approach holds great promise in accelerating the structure search and prediction of large metal clusters.

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B-130

Anharmonic Phonons and Anomalous Thermal Expansion in Vanadium Metal

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Vanadium, an important metal in the alloy and steel industry, exhibits very large thermal expansion behaviour at high temperatures. In this work, we have extensively identified the role of phonons in the anomalous thermal expansion behaviour of vanadium, particularly at high temperatures. We compared the different methods to evaluate the phonon anharmonicity, namely, the quasiharmonic approximation (QHA), and machine-learned force-field-based molecular dynamics (MLMD) simulations. At higher temperatures, the experimental thermal expansion coefficient continues to rise up to twice the QHA estimates, indicating significant anharmonicity. The MLMD, which includes all the anharmonic effects, successfully explained the anomalous expansion behaviour over 500-2000 K (shown in figure 1a). We used MLMD to calculate the spectral energy density of phonons up to 2000 K which reveal small phonon shifts but large broadening (shown in figure 1(b-c)). We compared this SED plots with the harmonic phonon dispersion as well as available measurement at 300K.We have highlighted the limitation of quasi-harmonic approximations (QHA) to predict the high-temperature thermal expansion behaviour in such a strongly anharmonic system.

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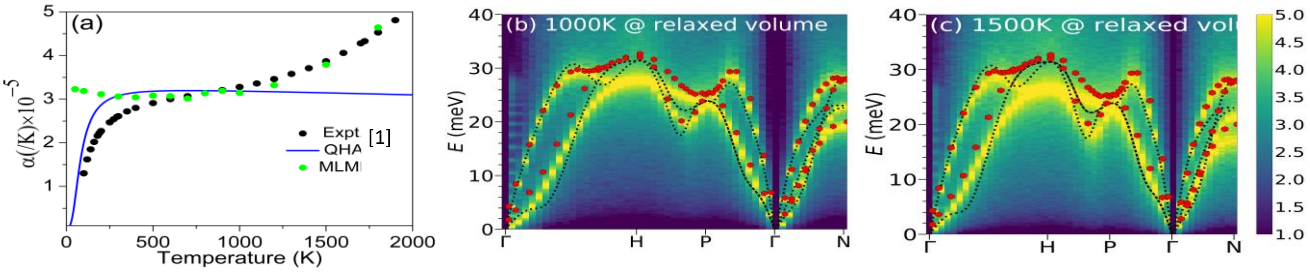

Figure 1: (a) The calculated thermal expansion coefficient of vanadium using QHA and MLMD simulations, compared with the available measurements [1], (b-c) The calculated phonon SED at 1000K, 1500K from MLMD simulations were compared with the available measurements at 300K (red circle) [2] and harmonic phonon dispersion (black dot lines) , highlights the phonon broadening and shifting effect.

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B-131

Graph Neural Network-based ML Models for Predicting the Yields of Cross-Coupling Reactions

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Catalysis represents one of the 12 principles of green chemistry. However, the high cost and inefficiency of catalysts for chemical reactions present significant barriers to the sustainable commercialization of these processes in synthetic chemistry. In this context, Artificial Intelligence (AI), particularly machine learning (ML), offers a promising solution by enabling more efficient, cost-effective, and sustainable alternatives. However, the potential of AI has not been explored much in this sector1. This study explores the application of AI, for predictive modeling of chemical reactions employing the Graph neural network models, paving the way for more efficient reaction optimization. Several GNN architectures were investigated, including Graph Attention Networks (GATs), Graph Convolutional Networks (GCNs), Graph Isomorphism Networks (GINs), and GraphSAGE, to predict yields in transition metal-catalyzed cross-coupling reactions. The dataset consisted of 4,825 diverse reactions catalyzed by metals such as Mn, Fe, Co, Cu, Zn, and Pd, which were pre-processed and encoded using molecular descriptors from RDKit, with chemical structures standardized in SMILES format. These structures were then converted into graph representations using k-nearest neighbors (KNN) for input into the GNN models. GraphSAGE achieved the highest predictive accuracy among the architectures tested, with an R^2 value of 0.72 on the test set. This result highlights AI's potential to reduce reliance on traditional experimental methods, accelerating the discovery and optimization of catalytic processes2. By aligning with sustainable development goals, this AI-driven approach provides a model for integrating advanced technologies into chemical practices, addressing both environmental and economic challenges, and guiding policy and governance toward more sustainable industrial processes.

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C-121

Electronic Structure Calculations of Th^{+4} ion adsorbed Modified Graphene Oxide

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Thorium is presently accruing considerable interest owing to its prospective significance across a range of disciplines, with particular emphasis on energy generation. A nationlike India, which possesseslimited uranium reserves, might regard thorium as a more viable alternative for acquiring energy security. In prior investigations, graphene oxide has been shown be an efficient sorbent for a variety of radionuclides, heavy metals, and precious metals, attributable to its porous architecture, substantial surface area and structural integrity. However, the influence of different oxygen-containing functional groups on graphene oxide, particularly the phosphate group, with respect to thorium adsorption has not been extensively investigated. To identify a highly selective and efficient sorbent for thorium, initial studies on interactions of Th^{4+}ions with various functional groups such as –PO$_4^{2-}$, -OH, and -O- attached to graphene oxide flakes have been performed using Density Functional Theory. The adsorption energies were computed for graphene oxide nano-flakes bearing a single functional group. For all the calculations VASP software (Version 5.4.4) was utilised.

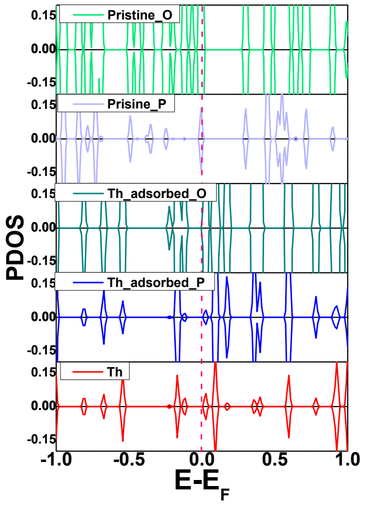

Figure 1. PDOS of oxygen and phosphorus in pristine structure and oxygen, phosphorus and thorium after Th^{4+} adsorption on functionalized graphene oxide

Three distinct modes of Th^{4+} adsorption on graphene oxide functionalized with single -PO$_4$, -OH, and -O- groups were investigated. Th^{4+} ions interact with the oxygen atom double-bonded to the phosphorus atom of the –PO$_4^{2-}$ group of graphene oxide, with an optimized bond distance of 2.21 Å. From adsorption energy calculation, the order of interaction of various functional groups of the phosphate modified graphene oxide with the Th^{+4} ions was obtained as -PO$_4$> -OH > -O- group. Fig. 1 shows the PDOS of O, P and Th^{4+} for pristine and thorium adsorbed graphene oxide.

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C-122

Predicting Stability Constants of Uranyl Complexes with Tri-Alkyl Phosphate Ligands

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It has long been debated whether the lanthanide/actinide extraction process can be accurately modelled using computations. This has been challenging because the process depends on many factors, such as the pH of the solvent, the properties of the chemicals involved, the concentration of the metal, the temperature, and the effects of radiation. About a decade ago, it was proposed that by calculating the free energy of complex formation, one of the most important experimentally determined thermodynamic quantities – the stability constant of the complex – could be predicted through computations [1]. More recently, it has been suggested that the accuracy of these predictions for new uranium and vanadium complexes can be improved by using known stability data from similar complexes, following a methodology outlined in Scheme 1 [2].

In this work, we applied quantum chemical calculations to investigate the electronic structure and complexation behavior of tri-alkyl phosphate ligands with shorter alkyl chains, ranging from methyl to butyl, with uranyl nitrate (1:2 complexes). The ORCA quantum chemistry program package [3] was used for these calculations, and charge and energy decomposition analyses were performed using NBO [4] and the Amsterdam Density Functional (ADF) program package [5], respectively. Based on the results, we set out to predict the stability constants for uranyl nitrate complexes with trialkyl phosphate ligands.

$$\begin{tikzcd}
{[M(H_2O)_m]^x}_{(gas)} \arrow[d, "{\Delta G^*_{solv}([M(H_2O)_m]^x)}"] & + & L^y_{(gas)} \arrow[r, "\Delta G^0_{gas}"] \arrow[d, "\Delta G^*_{solv}(L^y)"] & {[ML(H_2O)_{m-n}]^{x+y}}_{(gas)} \arrow[d, "{\Delta G^*_{solv}([ML(H_2O)_{m-n}]^{x+y})}"] & + & n\,H_2O_{(gas)} \arrow[d, "\Delta G^*_{solv}(H_2O)"] \\
{[M(H_2O)_m]^x}_{(aq)} & + & L^y_{(aq)} \arrow[r, "\Delta G^0_{solv}"] & {[ML(H_2O)_{m-n}]^{x+y}}_{(aq)} & + & n\,H_2O_{(aq)}
\end{tikzcd}$$

Scheme 1. Schematic representation of Born-Haber cycle to calculate change in Gibbs free energy.

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C-123

Computational Studies on *N*-Donor Ligands for Lanthanide Actinide Separation

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N-donor ligands are known to preferentially stabilize actinide complexes over lanthanide ones due to their greater polarizability and softer nature. As a result, they are explored as suitable ligands for the separation of lanthanides and actinides. The interactions between Am^{3+} and soft *N*-donor heterocycles are more covalent than those with Ln^{3+}, and it is believed that there is a stronger covalent interaction between these ligands and the 5*f* orbitals of the actinides compared to the 4*f* orbitals of the lanthanides. P. Y. Cordier, *et al.* [1] investigated the ability of 2,2′:6′,2″-terpyridine for the selective extraction of Am^{3+} from Eu^{3+}. Due to the high basicity of terpyridine ligand, the research focused on developing triazine-based ligands. M. J. Hudson *et al.* [2] identified bipyridine derivatives as potential candidates for An/Ln separation. However, despite the observed selectivity, these ligands resembled 2,2′:6′,2″-terpyridine in their extraction properties. Recently, Y. Xin *et al.* [3] reported the coordination chemistry of high-valent Am with *N*-donor ligands (tpy, dpp, BTP, BTBP, BTPhen) and recommended ligand design by modulating the redox potentials of hydrated Am(III) ions. Many of the above-mentioned *N*-donor chelators contain pyridine moieties. To illustrate their behavior, we used terpyridine as a representative ligand. Terpyridine forms stable coordination complexes with both *d*- and *f*-block metal ions, making it a prime example in the study of such ligands. In the present work, we first explored the various conformers of terpyridine to identify the most stable one (cf. Figure 1a). We also examined the transition states encountered during the optimization process and the corresponding molecular orbitals responsible for coordination with metal atom (cf. Figure 1b). For these analyses, we utilized the ORCA [4] quantum chemistry package.

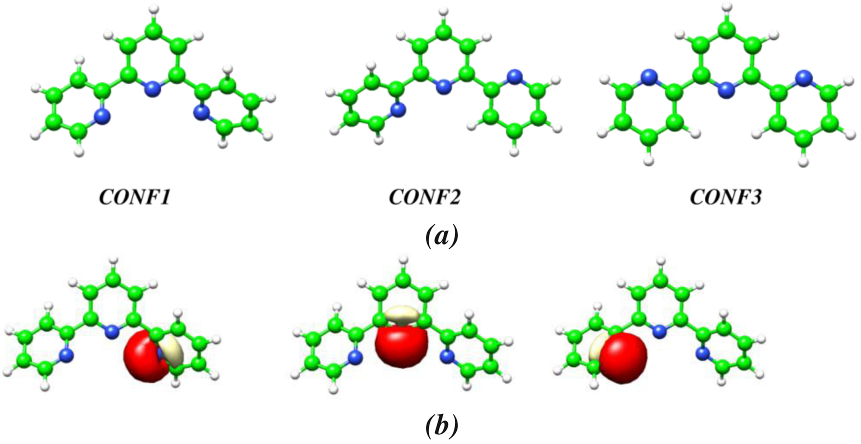

Figure 1. The DFT optimized geometries of 2,2′;6′,2″ -terpyridine conformers (a) and shapes of strongly localized molecular orbitals responsible for metal complexation (b).

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C-124

Understanding the Complexation Behaviour of Tri-n-Alkyl Phosphorotrithioate Ligands with Uranyl Nitrate

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In recent decades, soft donor atoms such as *N*- and *S*- atom substituted ligands have drawn significant attention due to their greater selectivity and affinity towards actinides over lanthanides [1]. However, the radiolytic and chemical stability of these ligands still needs to be verified through laboratory experiments. In this contribution, we investigated sulphur-substituted organophosphorotrithioate ligands, where the C-O-P unit is replaced by C-S-P [2]. The resulting ligands are tri-*n*-methyl phosphorotrithioate (TMPT), tri-*n*-ethyl phosphorotrithioate (TEPT), tri-*n*-propyl phosphorotrithioate (TPPT) and tri-*n*-butyl phosphorotrithioate (TBPT) [3]. The geometries and electronic structures of the respective complexes with uranyl nitrate were established (cf. Figure 1), and the calculated complexation energies were decomposed into various stabilizing (orbital interaction, electrostatic, dispersion energy) and destabilizing (preparation energy, Pauli repulsion) factors using the energy decomposition scheme implemented in the ADF 2016 program package [4]. The most significant stabilizing interactions were identified as dispersion contributions [TMPT (-28.0kcal/mol), TEPT (-34.2kcal/mol), TPPT (-41.7kcal/mol), TBPT (-59.1kcal/mol)] and orbital interactions [TMPT (-68.0kcal/mol), TEPT (-69.0kcal/mol), TPPT (-72.7kcal/mol), TBPT (-75.5kcal/mol)] [5].

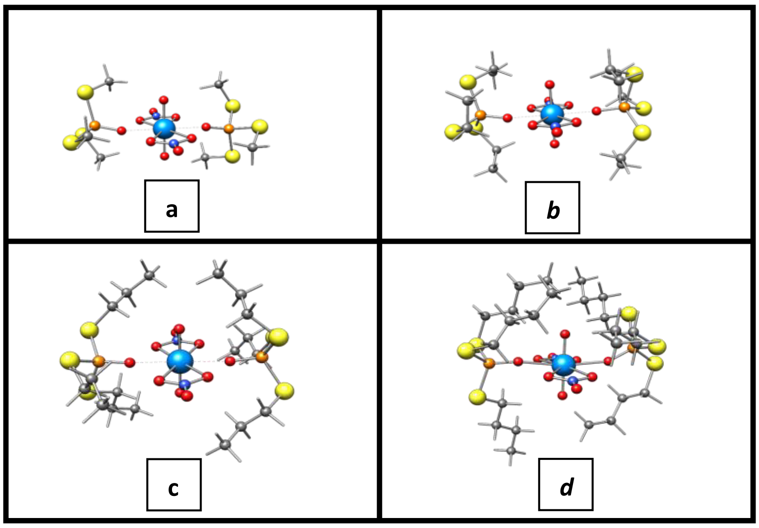

Figure 1. The DFT optimized geometries of (*a*) $UO_2(NO_3)_2$.2TMPT, (*b*) $UO_2(NO_3)_2$.2TEPT, (*c*) $UO_2(NO_3)_2$.2TPPT, and (*d*) $UO_2(NO_3)_2$.2TBPT.

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E-121

Structural and Thermodynamic Analysis of Polyaniline Mixtures in Oxidized and Unoxidized Form: A Molecular Dynamics Study

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Conducting polymers such as polyaniline (PANI) has shown a significant interest in the field of electrified membranes (EMs) with antifouling properties. EMs utilize charged or conductive polymers to prepare the membrane surface. These membranes may form electroactivity to mitigate fouling[1]. However, blending/doping of PANI with other polymers and nanomaterials highly influences the properties of the membrane surface [2]. PANI has both oxidized and unoxidized forms, namely, emeraldine salt (ES) and emeraldine base (EB), respectively. Therefore, understanding the PANI structure with the variation of the oxidized and unoxidized forms along the length of the polymer chain is Intriguing. In this work, we present the design of the novel copolymer consisting of EB and ES monomers with varying charge densities and arrangements.

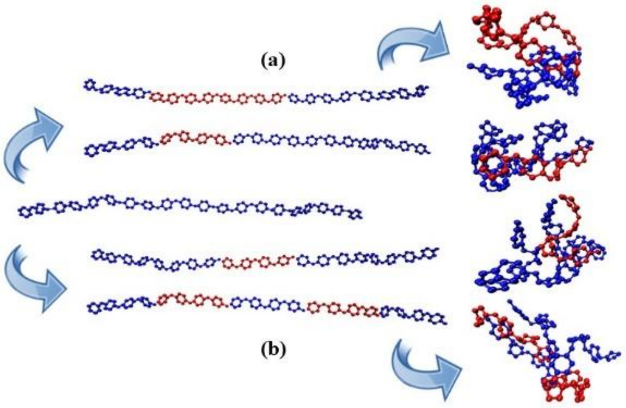

Fig. 1: Arrangements of the monomers in the polymeric chain with umbrella sampling (a) random and (b) sequential. Color code: Blue- EB and red-ES.

We present various intra and intermolecular structural properties of the PANI chain using molecular dynamics (MD) simulations. Our results show increased radius of gyration (R_g) values with the increase in charge density. Furthermore, we also present a detailed conformational free energy analysis to understand the PANI chain conformational transition.[4] H-bonding, spatial distribution functions (SDFs), and solvent accessible surface area (SASA) values lead to uncoiling and increased conductivity of the chain. These analyses are performed to understand the stability of different complex chains with unique arrangements. We observed the dependence of charge density on the behavior of the chains. Therefore, these observations are crucial in understanding the chains' complex behavior for designing anti-fouling electrified membranes. Intra- and intermolecular interactions are the main concern for the coiling behavior of the chain, which leads to gelation effects.

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E-122

Separation of 5-HMF from the Ionic Liquids Using Phenolic Solvents Using Molecular Dynamics Simulations

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To achieve a sustainable future to reduce global warming, there is a significant need for renewable energies such as solar, wind, geothermal, hydrothermal, and bioenergy[1]. Bioenergy derived from biomass has great attributes such as its abundant nature, and non-toxic to the environment. The feedstocks that are derived from the lignocellulosic biomass (LCB) are tangible to decrease greenhouse gases and found immense applications in the field of the production of fuels and value-added chemicals etc[2,3]. As per the Department of Energy, USA, 5-hydroxy-methyl-furfural (5-HMF) and other furfurals can be used in refineries and help generate biorefinery as well as green polymers, solvents, fungicides, and a range of chemical products[4]. Ionic liquids (ILs) are shown to be promising and very efficient in synthesizing 5-HMF from fructose. However, there is still a great challenge in separating the 5-HMF from the ILs. Various organic solvents are effective in separating 5-HMF from the Ils, as shown in Figure 1. However, 5-HMF can be extracted from ILs using organic solvents (hydrogen bond donors property) shown promising for the highly efficient extraction of 5-HMF[5].

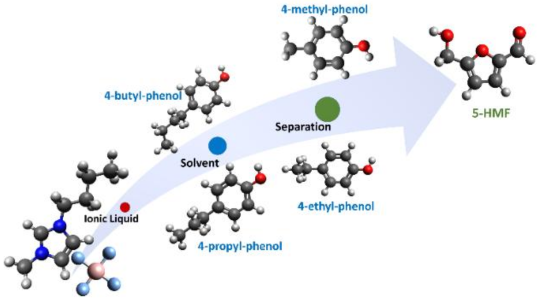

Figure 1. Separation of 5-HMF from IL using various organic solvents.

In this presentation, we aim to investigate various phenolic solvents that help in the effective separation of 5-HMF from ILs. We performed MD simulation by using GROMACS software and OPLS-AA force field. The geometry optimization is performed using density functional theory calculations at the level of B3LYP functional form and def2-SVP basic set using ORCA. We present various structural properties, interactions, dynamic properties, and separation thermodynamic properties. Our results show that the effective separation depends upon the role of the hydrophobicity of the solvent (4BP, 4PP, 4EP, 4MP). The self-diffusivity (D) of 5-HMF shows a decrease with an increase in the methyl group on the phenol. Due to the variation in the alkyl group on the phenols the oxygen atom of 4MP solvent shows a strong interaction with Solvent-$[BF_4]^-$ and solvent-$[BMIM]^+$. Interestingly we see higher mobility of the 5-HMF molecule due to the weak intermolecular interactions in the 4MP, thereby less solvation as seen from the solvation free energy calculations. Overall results obtained in this work were shown promising for the understanding of the complex interactions between furfural-based compounds and ILs for the separation of pure 5-HMF using an alkylated phenolic solvent.

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E-123

Gas Adsorption and Water Splitting Reaction in Ion-Exchanged Salts of Potassium Poly (heptazine imide) Two Dimensional Materials

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The potassium poly (heptazine imide) (K-PHI), a crystalline two-dimensional carbon-nitride material, is an active photocatalyst for water splitting. From powder X-ray diffraction data an idealized structural model of K-PHI has been derived, using this model we defined an energetically optimized K-PHI structure, in which the K ions are present in the pore and between the PHI-planes. The distance between the anion framework and K ion resembles a frustrated Lewis pair-like structure, which we denote as frustrated Coulomb pair that results in an interesting adsorption environment for otherwise non-adsorbing, non-polar gas molecules. We demonstrate that even helium gas molecules, which are known to have the lowest boiling point and the lowest intermolecular interactions, can be adsorbed in this polarized environment with an adsorption energy of -4.6 kJ/mol per He atom. The interaction between He atoms and K-PHI is partially originating from charge transfer, as disclosed by our energy decomposition analysis based on absolutely localized molecular orbitals. The potassium ions in K-PHI can be exchanged with other ions to change the properties of the material and eventually to design the catalysts. Here we report here the electronic structures of several ion-exchanged salts of K-PHI (K, H, Au, Ru, and Mg) and their feasibility as water splitting photocatalysts, which were determined by density functional theory calculations. The results are complemented by experiments where the performances in the photocatalytic hydrogen evolution reaction were recorded. We show that due to its narrow band gap, Ru-PHI is not a suitable photocatalyst. The water oxidation potentials are straddled between the band edge potentials of H-PHI, Au-PHI, and Mg-PHI; thus, these are active photocatalysts for both the oxygen and hydrogen evolution reactions, whereas K-PHI is active only for the HER. The experimental data show that these are active HER photocatalysts, in agreement with the DFT results.

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E-124

Redox Active Covalent Organic Framework based Two-dimensional Materials as Organic Electrodes in Alkali Ion Batteries

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Covalent organic frameworks containing carbonyl like redox active groups, crystalline and porous, two dimensional materials are promising candidates for organic electrodes in alkali ion batteries. However, the volume change, distortion of crystalline structures due to redox reaction are the main challenges, which are yet to be addressed. In this context, we studied an experimentally synthesized crystalline, porous and nitrogen rich redox active COF namely TQBQ (triquinoxaline benzoquinone) using density functional theory[1]. We first investigated the periodic structure of TQBQ-COF which is found to be in a hexagonal lattice with an inter-layer distance of 3.53 Å as illustrated in Figure 1. We then studied the interaction of alkali metal atoms (Li, N and K) with TQBQ using DFT and calculated various electrochemical parameters. The adsorption energies for Li, Na and K were in the range of -4.12 to -3.19 eV, -4.48 to -3.26 eV and -5.33 to -3.81 eV, respectively. A more negative interaction energy signifies a more favourable exothermic interaction between COF and metal atoms, allowing a greater number of AM atoms to be adsorbed. In total, a maximum of 72 AM atoms were adsorbed on the four-layered periodic TQBQ-COF. Further, we look into the more details of the interaction of AM atoms with TQBQ-COF, our point charge analysis clearly suggests that the charge transfer from the AM atoms to TQBQ. The average voltages observed are in the range of 4.12 - 3.18 V, 4.48 - 3.69 V and 5.32 - 3.32 V for Li, Na and K, respectively. The highest average voltage is obtained for the potassium ion owing to corresponding large interaction energy. Further, we found the total volume change decreases due to addition of AM atoms because of increased interaction between the layers due to charge transfer. However, the change in total volume is less than 20% in this material due to insertion of K-ions with a marginal change in the lattice parameters even in the interlayer distance. Our results indicate that TQBQ-COF will be best suited for a potassium ion battery with higher voltage and minimal change in the volume [2].

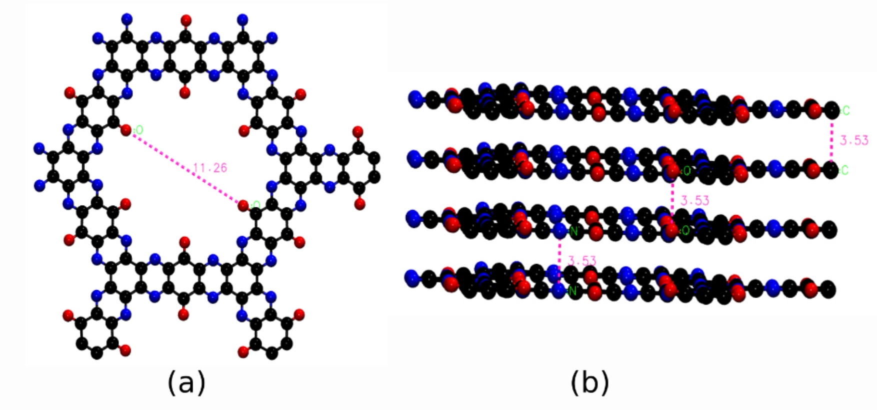

Figure 1. The DFT-optimized bulk structure of TQBQ-COF (a-top view and b-side view) in a hexagonal lattice. Atoms color: C-black, N-blue and O-red.

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E-125

Nonpolar Surface in Wurtzite CdS Quantum Dots Enhances the Charge Separation and Carrier Lifetime in CdS Quantum Dots/Graphene Nanoribbon Nanohybrid

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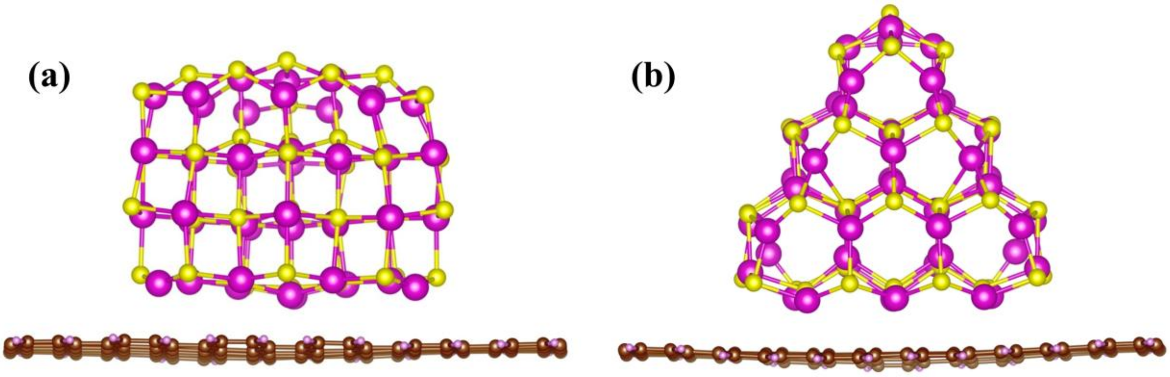
Different physical and chemical properties of polar and nonpolar surfaces of quantum dots (QDs) have a significant role in the optoelectronic and photocatalytic applications. Therefore, employing nonadiabatic molecular dynamics theory within the tight-binding approach [1], we investigate the photoinduced carrier dynamics of wurtzite cadmium sulphide (CdS) QDs/ graphene nanoribbon (GNR) nanohybrids system to explore the role of surface polarity. Wurtzite CdS QDs form noncovalent composites with GNR through polar (c-plane [0001]) and nonpolar surface (a-plane [$11\bar{2}0$]), shown in Figure1a,b. Our simulations demonstrate that ultrafast hole transfer (HT) is accelerated up to 2 times and exciton life time is enhanced nearly 8 times in nonpolar CdS-QDs/GNR compared to polar composite without hampering the ultrafast electron transfer (ET). The simulated charge transfer time scales are excellently corroborated with the experiment [2]. We explained that ultrafast ET occur from CdS-QDs to GNR due to strong nonadiabatic coupling (presence of mixed states), large energy offset and long-lived quantum coherence presence between donor and acceptor states in both nanohybrids. In case of HT, nonpolar CdS-QDs/GNR exhibits stronger nonadiabatic coupling, longer quantum coherence and involvement of broad range of electron-phonon vibrational modes compared to polar CdS-QDs/GNR. Hence HT is twice faster for nonpolar CdS-QDs/GNR. On the other hand, in nonpolar CdS-QDs/GNR, overlap of electron and hole wave functions are significantly reduced by the potential polarization which directly reduces the rate of electron-hole (e-h) recombination [3]. Further, high average energy gap, separated spatial distribution of charge and weaker nonadiabatic coupling slow down the e-h recombination. The time-domain quantum dynamics simulations explore that the photoinduced charge transfer is strongly governed by the surface polarity and provide new insight for improvement of energy conversion performance.



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E-126

Improvement of Photocatalytic Activity of TiO_2 for H_2 Generation and CO_2 Reduction: A DFT Study

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This study investigates the possibilities of enhancement of photocatalytic activity of TiO_2 for hydrogen generation and carbon dioxide conversion under visible light irradiation, which are emerged as two appealing alternatives aimed at mitigating global warming and fostering the production of sustainable energy. [1] The objective of maximizing the utilization of sunlight for these purposes has sparked an interest for efficient materials, driving researchers to study the electronic structure of TiO_2 in anatase phase. Building on experimental observations, we investigated the potential impact of doping anatase with Cu followed by codoping Cu-doped TiO_2.

Spin polarized computations have been carried out utilizing the Vienna ab initio simulation package (VASP). The electronic structure analyses were exclusively performed employing the HSE hybrid density functional.

Pure TiO_2 (Figure 1(a)) exhibits a bandgap of 3.13 eV, limiting its photocatalytic activity to UV region of the spectrum. The band structure for Cu-doped TiO_2 shows discrete unoccupied midgap states which divide the band gap into two regions (0.96 eV and 1.75 eV). The impurity states reduce the effective band gap for excitation of electron. Unfortunately, these states accelerate the rate of electron-hole recombination, resulting into reduction in photoconversion efficiency. Interestingly, doping TiO_2 with W and Mo completely passivates the impurity states, resulting into formation of clean band structure depicted in Figure 1(b) and Figure 1(c), which ensures enhanced photoconversion efficiency attributed to the extended light absorption and reduced recombination of photogenerated electron-hole pairs.

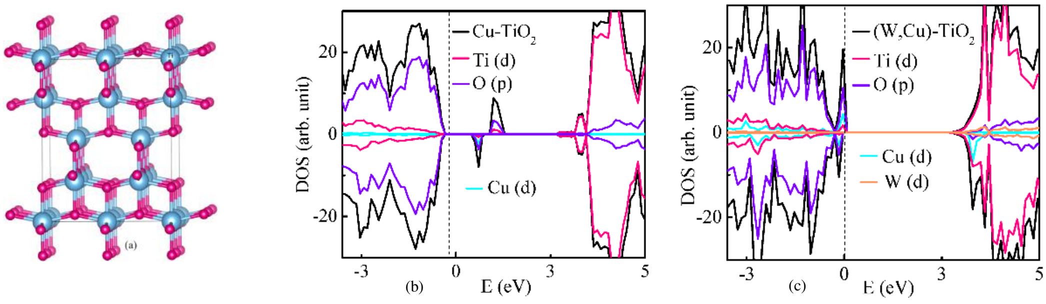

Figure 1: (a) 2 × 1 × 1 supercell structure of cubic TiO_2. (b) DOS plot for Cu-TiO_2. (c) DOS plot for (Cu,W)-TiO_2.

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E-127

Site Specific Descriptor for Metals for Oxygen Evolution Reaction Activity on Single Atom Catalysts Using QMML

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Descriptors are properties or parameters of a material that is used to explain the any catalytic activity both computationally and experimentally. Such descriptors aid in designing the materials property to obtain efficient catalyst. d-band center, given by Hammer and Norskov in 1995, explained the binding strength of oxygen atom on pure transition metals [1]. For transition metals, d-band center is a well-known descriptor that shows Sabatier type relation for several catalytic reactions. It is well known that, when the dimensions of a system are lowered the states become narrow and localized. In such systems, the d-band center does not explain the catalytic activity well and it is an open research problem [2]. Studies reveals the d-band center works well for metals across the group under same electronic environment (facets, substrate, phase, etc.,) but fails for a same metal under varying conditions and in nano dimensions. Following the criteria of localized states, single atom catalysts (SAC) are the materials, where the metal atom states are localized. Low dimensional carbon has been used as the host for SAC and extensively studied towards several catalytic reactions. Some of these syntheses involves the use of organic polymers instead of graphene as precursor material have made synthesis and structural engineering possible. In the carbon class, the graphene nanoribbons (GNRs) with width variation and doping make them good support for SACs. SAC on GNRs could be used to test the impact of GNRs on electronic properties of SAC and obtain multiple electronic parameters that can be utilized in machine learning to do a deeper search for a better descriptor that could explain as well as predict the catalytic activity. To address this, density functional theory was used for single atom catalysts (SACs) [2] embedded on armchair and zigzag graphene nanoribbons (AGNR and ZGNR). By varying the anchoring nitrogen atoms' orientation and considering pristine and doped cases 432 active sites were used to test the oxygen evolution reaction [3] activity. It was observed that S and SO_2 dopant helps in reducing the overpotential on Co-SAC ($\eta = 0.28$ V). Along with the d-band center, a total of 105 possible descriptors were tested individually. Machine learning process were employed to narrow down unique descriptors and several algorithms were trained on the two obtained descriptors. Among the models, support vector regression model showed highest performance with $R^2 = 0.89$ on test data. This work shows the necessity of a multi-descriptor approach to explain OER catalytic activity on SAC and the approach would help in identifying similar descriptors for other catalytic reactions as well.

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E-128

Optimizing Sodium-Ion Batteries through LHCEs in Organic Carbonate-Based Electrolytes

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Sodium-ion batteries (SIBs) hold significant promise for large-scale energy storage applications. However, their performance is critically dependent on the electrolyte's ability to facilitate rapid ion transport while maintaining a stable electrode-electrolyte interface. Localized high-concentration electrolytes (LHCEs) have emerged as a promising approach due to their enhanced ionic conductivity and solid electrolyte interphase (SEI) formation [1]. This study employs first-principles calculations to investigate the solvation structure and stability of carbonate-based LHCEs for SIBs. Specifically, we investigate sodium bis(fluorosulfonyl)imide (NaFSI), ethylene carbonate (EC), propylene carbonate (PC), and 1,1,2,2-tetrafluoroethyl-2,2,2-trifluoroethyl ether (TTE) as diluent. We examine the evolution of solvation complexes from dilute to high-concentration regimes, elucidating the role of salt concentration on electrolyte structure and the influence of diluent in localized high-concentrated electrolytes. The ion solvation/desolvation study of the electrolyte identifies 2PC/EC/TTE-NaFSI as an optimal LHCE formulation. We relate the structural changes to the electronic properties of the electrolytes, finding a relationship between the reductive behavior of the solvated complexes. The reduction potential of 2PC/EC/TTE-NaFSI is enhanced to 0.27 V compared to the HCE formulation. Additionally, the lowest unoccupied molecular orbital (LUMO) analysis suggests that TTE facilitates the reduction of the FSI^--anion. We conducted the comparison using $NaClO_4$ as the metal salt. However, there was no decrease in the anion molecule, verifying the non-film-forming characteristics of $NaClO_4$. In contrast, solvation shells containing FSI^--anions are reduced to form an interphase film, which can enhance the durability and rate capability of the cell. The solvation/desolvation model reveals that the electrolytes containing NaFSI can achieve a faster Na^+ desolvation process compared to $NaClO_4$-based electrolytes [2]. The solvated ion structure in HCE and LHCE demonstrates the potential of carbonate-based electrolytes to surpass current limitations, thus enhancing the performance of sodium-ion batteries.

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E-129

Cation-π Interactions Involving Graphynes: An Intermolecular Force Field Formulation

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An accurate description of potential energy surfaces governing cation-π interactions using empirical potentials is imperative for large-scale simulations involving materials and biomolecules [1, 2]. The current study proposes empirical intermolecular potentials for describing the interactions of alkali metal ions such as Li^+, Na^+, and K^+ with graphene and graphynes (GYs). GYs are 2D allotropes of carbon with both sp and sp^2 carbon atoms. GYs are classified as GYNs based on the number of acetylenic linkages between two sp^2 carbons (N). Herein, we present an intermolecular force field formulation for the description of cation-π interactions involving alkali metal ions (Li^+, Na^+, and K^+) and γ-GYs (γ-GYN; N = 1-4). We use Lennard-Jones (LJ) and improved Lennard-Jones (ILJ) potentials [3, 4] along with the Coulombic potential to describe the cation-π interactions. The potentials are parametrized by considering the potential energy profiles generated using density functional theory (DFT) as the benchmark. The benchmark DFT calculations are carried out using Gaussian 16 software [5]. The potential energy profiles corresponding to the motion of ions through the triangular pore of GYs and above the hexagonal pore of graphene are chosen for the investigation. We have adopted a weighted root-mean-square (RMS) deviation of the empirical potentials from the DFT potentials as the objective function to parametrize the empirical potentials [6]. The parametrization is done using an in-house developed Python script. The minimization is implemented using a second-order optimization algorithm available in the SciPy library, namely, limited-memory Broyden-Fletcher-Goldfarb-Shanno (L-BFGS) algorithm [7]. In addition to revealing the role of electrostatic interactions in describing cation-π interactions between alkali metal ions and various GYs and graphene, the current study provides an empirical approach that can be employed in large-scale simulations for applications in batteries, energy storage etc.

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E-130

First Principle Tailoring of Metal Porphyrins for Electrocatalysis

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Porphyrins are a group of cyclic tetrapyrrolic compounds with four pyrrole subunits interconnected via methine bridges. The heterocyclic structure is a largely conjugated aromatic ring; that can in principle bind almost all metal ions to produce a four-coordinated structure. In nature, metalloporphyrins are involved in a wide variety of important biological processes, for example, hemoglobin and myoglobin. Metal porphyrins present an ample scope for tailor made application by modification of coordination environment of metal. This can be attained by addition of different types of ligands and modulation of electron and proton distribution by attaching acid/base groups on porphyrin group. The talk will highlight our density functional studies on Cobalt Porphyrin (CoPr) to design an efficient electrocatalyst for Oxygen reduction and evolution reactions (ORR/OER) that hold the potential as the means to provide sustainable energy solutions. Both reactions use precious metal-based electrocatalysts that are limited and expensive making a strong case to develop low-cost, active and stable electrocatalysts. Tailoring of CoPr framework by introducing meso phenyl substituents in the Pr ligand and further substitution of phenyl group by ortho/para-anilino groups resulting CoTPP, CoTPP-o-NMe3, and CoTPP-p-NMe3 catalysts. Computational free energy profiles were constructed for each catalyst to elucidate the influence of peripheral substitution on the overpotential. Our results demonstrate that CoTPP-o-NMe_3 exhibits remarkable bifunctional electrocatalytic activity toward both ORR and OER, with overpotentials of 0.45 eV and 0.28 eV, respectively. Notably, the ORR performance of CoTPP-o-NMe_3 is on par with that of Pt, while its OER activity surpasses those of benchmark Ir- and Ru-based catalysts.

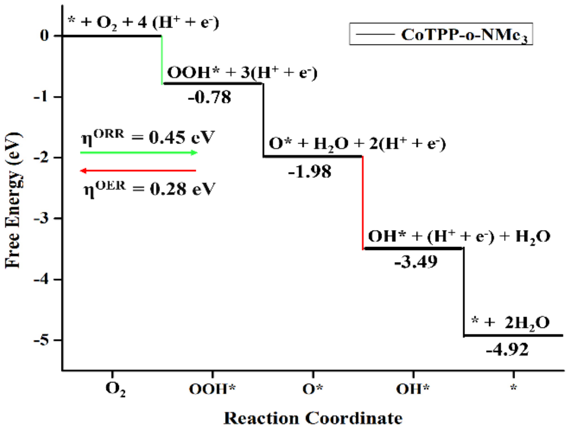

Figure 1. ORR and OER reaction free energy profile on CoTPP-o-NMe_3.

E-131

N-Doped Biphenylene Monolayer as High-Performance 2D Electrode Material for Li-Ion Batteries

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Incorporating heteroatoms into the two-dimensional lattices of materials like biphenylene leads to groundbreaking advancements in material science, imparting extraordinary properties to the base material [1]. In this study, a two-dimensional carbon lattice doped with nitrogen atoms as demonstrated in Figure 1(a), known as N-doped biphenylene (N-BPN), has been explored [2]. Its potential utilization as an anode in secondary lithium-ion batteries (LIBs) has been showcased. Density Functional Theory (DFT) computations reveal that the N-BPN monolayer possesses a stable composition that remains resilient under dynamic, thermal, and mechanical conditions, exhibiting consistent metallic properties. The density of states study validates the monolayer's metallic properties, further enhancing its suitability for utilization as an electrode. The mean adsorption energies for consecutive adsorption of the lithium atom onto the monolayer were found to vary between −0.91 to −0.20 eV, leading to a transfer of 0.87e from lithium to the monolayer. N-doped monolayer offers a minimal migration barrier of 0.20 eV and an elevated diffusion coefficient of 4.18×10^{-5} cm^2s^{-1}. The migration of Li-ion onto the monolayer suggests an active charge/discharge process. N-BPN monolayer attained a high storage capacity of the order 1447.5 $mAhg^{-1}$, and a low working voltage of 0.25 V as shown in Figure 1(b), and extremely high energy densities of 4038.5 $mWhg^{-1}$. In light of the collective findings of this study, it is evident that the N-BPN monolayer shows significant promise for serving as electrode material in LIBs for further generations.

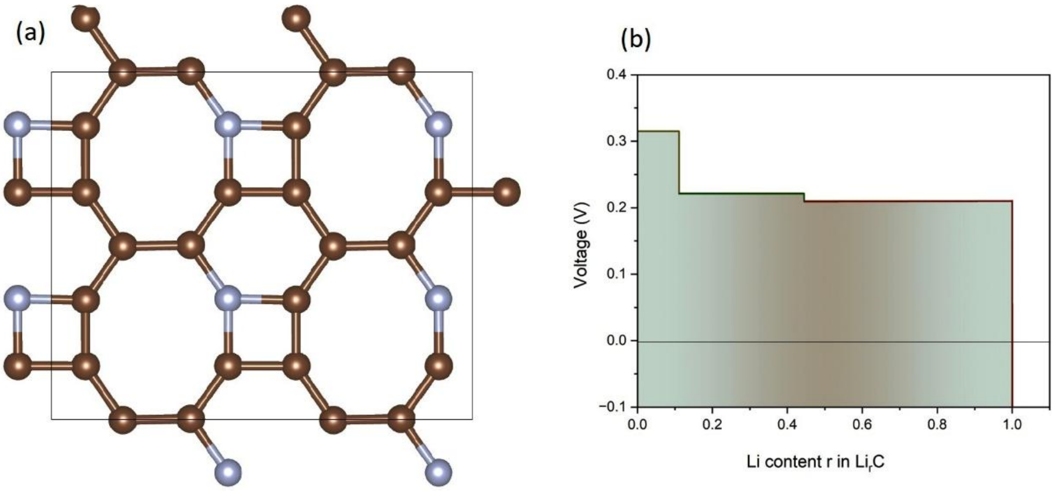

Figure 1. (a) Relaxed geometry of 2 × 2 × 1 N-doped biphenylene supercell, and (b) the voltage plateau pattern corresponding to different concentrations of Li ions.

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E-132

Exploring 1D MOFs as Single-Atom Catalyst for Oxygen Evolution Reaction/Hydrogen Evolution Reaction: A DFT Study

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Energy plays a vital role in the advancement of science and technologies. With the boost in quality of human lifestyle and heightening of the technological dependence, the energy demands are rapidly increasing. Clean, renewable energy sources have gained significant importance lately due to the limited availability of traditional energy resources and their adverse environmental impact. Hydrogen is considered as the fuel for the future. Amongst the various routes of hydrogen production, electrolysis of water is considered to be one of the cleanest routes. In an electrolyzer, the cathode and anode reactions are hydrogen evolution reaction (HER) and the oxygen evolution reaction (OER) respectively. Pt and Pt-based catalysts are most commonly used for HER, whereas Ir and Ru-based catalysts are used for OER. The major drawback with these catalysts is their limited abundance which makes them costly [1]. In the current study, the electrocatalytic activity of one-dimensional π-d conjugated conductive metal organic frameworks (MOFs) towards OER and HER is examined using density functional theory (DFT) studies [2, 3]. Here we considered Co, Ni, Cu and Zn based MOFs and optimized the structures and the same for Co-MOF is shown in Figure 1(a). Among the series, Co-MOF is found to be the better candidate. The free energy plot for OER in acidic medium for Co-MOF is shown in Figure 1(b). Further to fine-tune the catalytic activity through modulating the electronic structure of the active site, functionalization of Co-N_4 unit by phenyl (electron withdrawing) and methyl (electron donating) groups are studied. It is observed that phenyl-functionalized Co-BTA shows enhanced catalytic activity for OER with an overpotential value of 0.16 V. Functionalization with an electron-donating substituent (methyl) is found to significantly enhance the HER activity with a 10 times lower free energy change for H adsorption as compared to that in pure Co-BTA.

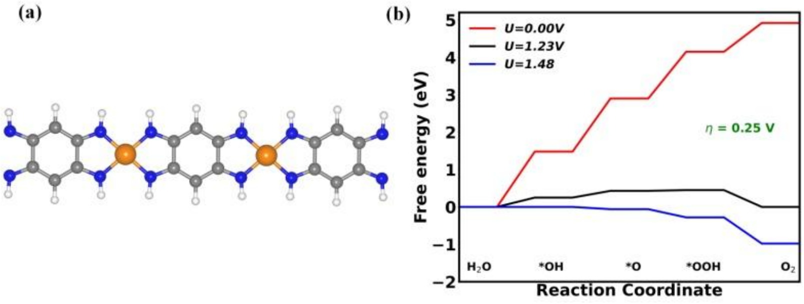

Figure 1. (a) Optimized structure of Co-MOF and (b) Free energy plot for OER in Co-MOF

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E-133

Molecular Engineering of Donor and Acceptor Moieties in Zn-Porphyrin Dyes for Dye-sensitized Solar Cells

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A thorough investigation was carried out on a range of Zn-porphyrin sensitizers using both static and time-dependent density functional theory calculations to identify highly efficient candidates for dye-sensitized solar cells (DSSCs). The SM315 dye, known for achieving a record-breaking power conversion efficiency of 13%, served as the reference. This dye features a bis(2',4'-bis(hexyloxy)-[1,1'-biphenyl]-4-yl) amine donor (D0), a phenyl ring as the π-linker bridge, and a carboxylic acid as the acceptor (A0). Eleven electron-rich donor groups (D1-D11) and four electron-withdrawing acceptor groups (A1-A4) were incorporated to optimize its design. The performance of these in silico designed sensitizers was tested in a simulated solar cell setup using a TiO_2 semiconductor and I_3^-/I^- electrolyte. Most of the modified dyes exhibited red-shifted absorption spectra. FMO analysis (Figure 1) reveals that the engineered dyes SM-D9-A1 to SM-D9-A4 exhibit a narrow band gap and their frontier molecular orbitals were well-aligned with the semiconductor's conduction band suggesting favourable electron injection and dye regeneration. Key efficiency metrics such as light-harvesting efficiency (LHE), short-circuit current density (J_{SC}), open-circuit voltage (V_{OC}), exciton binding energy (EBE), reorganization energy (λ), electron transfer rate (k), and polarizability and hyperpolarizability (α and β_{tot}) were analysed relative to the SM315 dye. Notably, the dye modified with a D9 donor group and A1-A4 acceptor groups achieved a remarkable power conversion efficiency exceeding 29%. This study not only proposes the design of a highly efficient porphyrin sensitizer at the molecular level but also provides a detailed understanding of its impact on DSSC performance through advanced analysis.

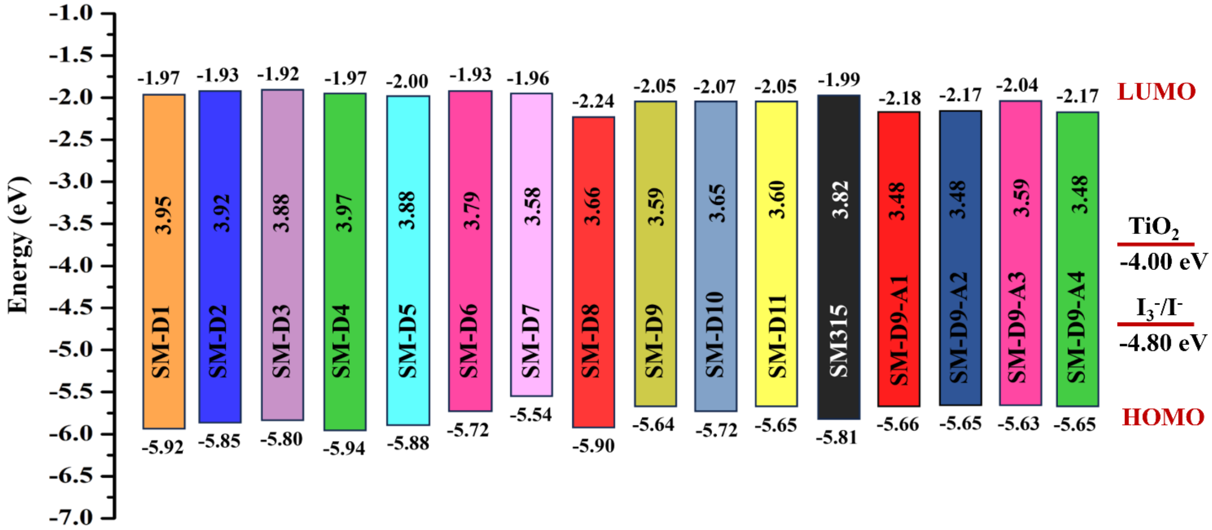

Figure 1. Molecular orbital energy levels and band gap of the tailored dyes.

E-134

Enhancement of Luminescence Characteristics of $ZnAl_2O_4$ Via Dopant Manipulation

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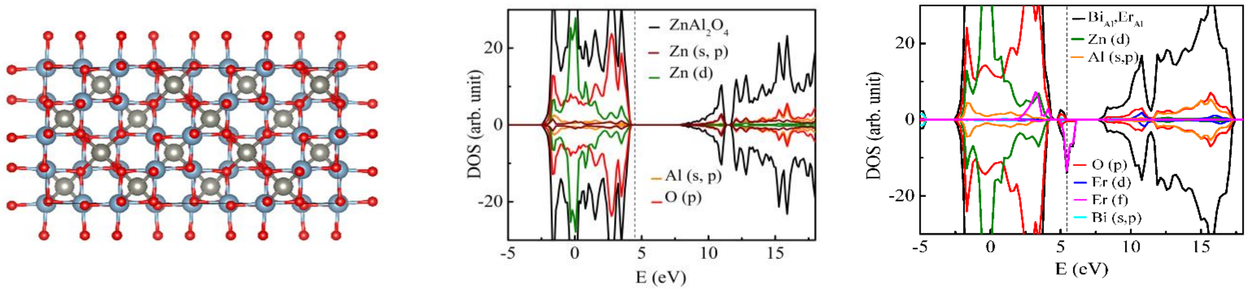
The incorporation of certain dopants in solid-state materials plays a crucial role in modifying their electrical, optical and structural properties. $ZnAl_2O_4$ is acknowledged for its versatility with distinguished attributes such as wide band gap, exceptional thermal stability, chemical resilience and luminescence. Nevertheless, its wide band gap energy restricts its applicability to UV region only. Driven by experimental findings [1], the present investigation underscores the significance of erbium (Er) and bismuth (Bi) as dopants in modifying the band gap energy and luminescent properties of $ZnAl_2O_4$.

The computational approach employed in this research were performed utilizing Vienna ab initio simulation package (VASP) along with projector augmented wave (PAW) pseudo potentials for Density functional theory (DFT) calculations.

The band gap energy of pure $ZnAl_2O_4$ (Figure 1(a)) is 3.84 eV as shown in Figure 1(b). The preference of dopant site is investigated through formation energy calculations. Initially, erbium is introduced as a single dopant. The formation of trap state between VBM and CBM is primarily accountable for reduction in band gap energy. However, the introduction of trap state leads to increase in the rate of electron-hole recombination, consequently decreases the efficiency of the emitted radiation. Then, bismuth is co-doped in the Er-$ZnAl_2O_4$ crystal lattice. Co-doping bismuth results in the formation of significantly narrower trap state compared to singly doped $ZnAl_2O_4$ as observed in Figure 1(c). As a result, the band gap energy get reduced and the electron-hole recombination rate decreases, leading to enhanced efficiency of emitted radiation. Therefore, it can be concluded that co-doping of bismuth emerges as more advantageous approach for enhancing luminescent characteristics of $ZnAl_2O_4$ compared to singly doped erbium.



(a) **(b)** **(c)**

Figure1: (a) 2 × 1 × 1 supercell structure of $ZnAl_2O_4$ (b) DOS plot for $ZnAl_2O_4$ (c) DOS plot for (Er_{Al},Bi_{Al})-$ZnAl_2O_4$.

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E-135

From NHC to Conjugated NHC Boryl Anions: Revolutionizing Hydrogen Activation

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Dihydrogen (H_2) plays a pivotal role in catalytic processes such as hydrogenation and organic transformations, and is increasingly recognized as a potential energy storage medium. Traditional transition metal complexes have been extensively studied for H_2 activation due to their ability to facilitate the cleavage of the H-H bond. However, the search for more efficient, cost-effective, and environmentally benign catalysts has shifted attention towards organometallic and main-group chemistry [1-3]. N-Heterocyclic Carbenes (NHCs) have emerged as versatile ligands in coordination chemistry, known for their strong σ-donating and weak π-accepting properties. These characteristics make NHCs excellent catalyst and stabilizers of metal centres, enabling diverse catalytic transformations [4-6]. Recent advancements have extended this research to doped analogues, such as N-Heterocyclic Boryl anions (NHBs), which incorporate boron atoms into the carbene framework. NHBs introduce unique electronic and steric properties that can potentially enhance catalytic activity and selectivity [7,8].

This study investigates and compares the catalytic efficacy of NHC and NHB in the activation of molecular hydrogen (H_2), with a focus on the effects of electron-donating and electron-withdrawing functional groups at the nitrogen atom. Additionally, the impact of conjugation on NHB in H_2 activation is explored (Figure 1). The computation was performed using Gaussian09 software package with the M06-2X / aug-cc-pVDZ level of theory. In addition to structural and electronic analysis of the reaction points, the catalytic reaction mechanisms were also explored, revealing key factors that influence catalytic performance. These insights contribute to the design of more efficient catalysts for hydrogen-related applications, promoting advancements in sustainable chemistry and energy storage. The detailed results evolved from the study will be presented in the proposed poster.

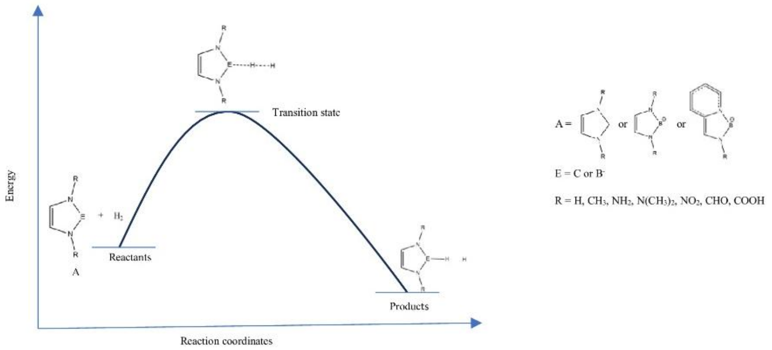

Figure 1: Reaction coordinates diagram of H_2 activation

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E-136

Conversion of Primary Alcohol to Ester in Presence of Ruthenium(II)-PNP Pincer Complex and Comparison with Isoelectronic (PNP)Os and (PNP)Rh$^+$ Complexes: A Computational Study

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Ester-based fuels represent a viable renewable fuel choice for the aviation, marine, and road transportation industries. They are also useful for reducing emissions of greenhouse gases. Esters serve as a readily available precursor for the preparation of organic compounds with different functionalities, viz., alcohol [1], amide [2] etc. In the present venture, mechanistic pathway of (PNP)Ru{PNP=bis[(2-*dimethylphosphino*)-*ethyl*]amine}mediated synthesis of an ester (2-methoxyethyl-2-methoxyacetate) from two equivalent of a primary alcohol (3-oxabutanol) is investigated using Density Functional Theory(DFT).

The complete catalytic cycle, depicted in Figure 1, is observed to be multi-step. The reaction commences with the 1:1 precursor complex formed between a molecule of alcohol and the pincer complex, whose intra-molecular decomposition leads to one equivalent of aldehyde and H_2 each. Then the second alcohol molecule takes part in a coupling reaction with the aldehyde, which eventually results in the formation of the ester and the second H_2 molecule. Two isoelectronic pincer complexes, (PNP)Os and (PNP)Rh$^+$, are also considered to shed light on the variation of the energetics with the change in metal-center of the catalyst. The overall reaction for all the three complexes is found to be slightly endergonic, indicating the requirement of a slightly high temperature. Theoretical catalytic efficiency and TOF values infer that the complex, (PNP)Ru, behaves as the best candidate among the three pincer complexes considered.

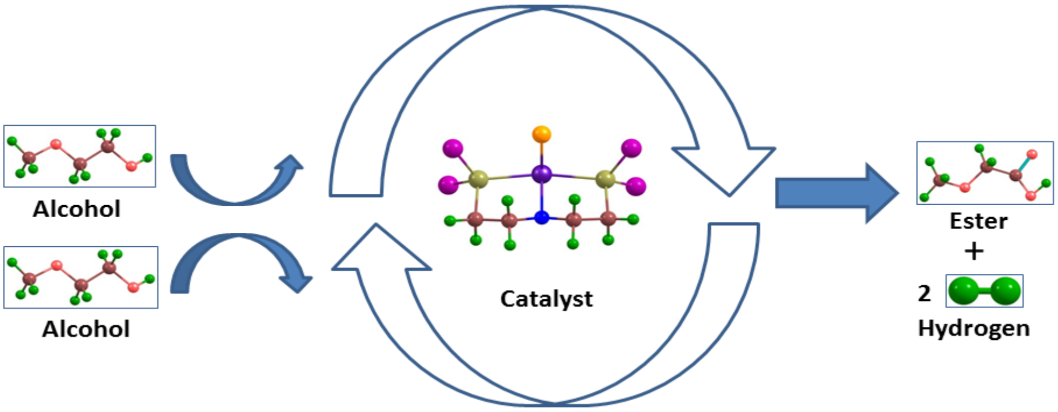

Figure 1. Reaction Scheme of (PNP)Ru (C1) catalysed ester (E) synthesis from alcohol (A) with removal of two equivalents of hydrogen.

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E-137

Immobilization of Cellulase Enzyme on Single-Walled-Carbon Nanotube for Recycle of Enzyme and Better Yield of Bioethanol using Computer Simulations

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The utilization of microbial cellulase enzymes for transforming plant biomass into biofuel or bioethanol, which can serve as a substitute for fossil fuel, is a subject of growing interest. Nonetheless, large-scale production of biofuel using cellulases is not economically feasible as extraction of these enzymes from diverse microorganisms is an expensive process. To address this issue, immobilizing the enzyme to a substrate material, e.g. carbon nanotube (CNT), to recycle without significant decline in its catalytic activity is a promising solution. Due to the hydrophobic nature of CNT, we employed molecular docking and network analysis methodologies to identify potential CNT-binding sites on the outer surface of a wild-type cellulase enzyme, CelS. Classical molecular dynamics simulations of CNT-bound CelS through one of the selected binding sites resulted in negligible changes in the secondary structure of the enzyme and its catalytic domain implying a least possible effect on the catalytic activity post-immobilization. Furthermore, our study reveals that while the unfolding near the CNT-binding region in CelS is more pronounced when the enzyme is interacting with wider CNT, resulting in enhanced contact area and improved binding affinity, its impact on the overall CelS structure is relatively less significant when compared to thinner CNTs. Particularly, CNTs of diameter ~12Å can serve as a favorable option for substrate material in cellulase immobilization. Our study also provides critical insight into the binding mechanisms between cellulase and CNT, which could lead to the development of more efficient biocatalysts for biofuel production.

E-138

Tuning Coordination Environment of Single-Atom Doped MoX_2 Monolayer for Enhanced Hydrogen Evolution Reaction: A DFT Study

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Hydrogen evolution reaction (HER) is an efficient technology for producing hydrogen and as a renewable energy carrier.[1] However, the effectiveness depends on the efficiency and cost-effectiveness of the catalyst. Recently, 2D transition metal dichalcogenides (TMDC) was found to be a promising candidate for electro-catalytic reactions.[2] In this study, we tuned the properties of the catalyst by doping non-metal atoms such as boron, carbon, and nitrogen family elements on the chalcogen vacancy of a defective MoX_2 (X = S, Se and Te) monolayer (shown in Figure 1) to determine the best candidate for HER. Using the dispersion-corrected density functional theory (DFT-D3) method, we screened all the single-atom catalysts (SACs) for HER activity.[3,4] The stability of single atoms doped at chalcogen vacancy of the MoX_2 monolayer was found to be stable in terms of binding energy. From the Gibbs free energy calculations, among the studied SACs, we found that B-$MoSe_2$, Sn-$MoSe_2$, B-$MoTe_2$, and Sn-$MoTe_2$ monolayers show promising performance for HER. Our DFT simulations reveal that tuning the coordination environment around the active site plays an important role in controlling the catalytic activity and selectivity. This work provides systematic views on the design of materials for HER through water splitting.

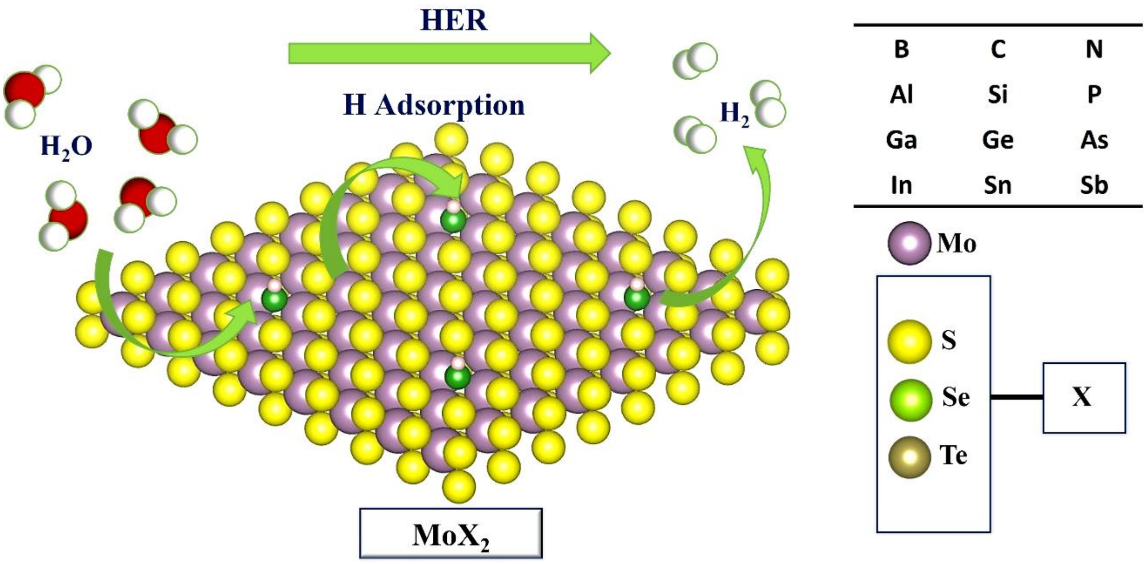

Figure 1. Graphical representation of Hydrogen Evolution Reaction for $BMoX_2$ SAC.

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E-139

Molecular design of porphyrin dyes with π-bridge for use in dye-sensitized solar cells: A DFT approach

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Dye-sensitized solar cells (DSSCs) have been explored for low manufacturing costs, ease of fabrication, tunable color and transparency features. Porphyrin, a dye with structural similarities to chlorophylls, requires special mention due to their exceptional photophysical properties and electrochemical stabilities. In the present study, density functional calculations (DFT) have been utilized to shed light on the HOMOLUMO energy gap of previously synthesized dye NiTPP-CA, cyano-3-(2′-(5′,10′,15′,20′tetraphenylporphyrinato nickel (II)) cyano-acrylic acid and it has been found that the HOMO-LUMO energy gap of this dye was 2.08 eV. Further we have modified its acceptor groups to minimize the energy gap for fast charge transfer. Fig. 1 represents the modification in acceptor group.

This proposition is tested by inserting thiophene or furan rings into the β-substituent of NiTPP-CA to form new analogues. These computationally designed dyes have modest band gaps (1.9eV-2.4eV) in comparison to our current base sensitizer, NiTPP-CA (2.54 eV). They also have wide absorptions with strong oscillator strengths at porphyrin Q bands, which are evident from TD-DFT studies. It may be concluded that the modified acceptor units of the new dyes render their stronger electron withdrawing ability with respect to NiTPP-CA, which in turn has resulted better charge transfer. Our computational studies will provide new insight for the design and screening of high-efficiency porphyrin dyes for DSSCs applications for enhanced light harvesting processes.

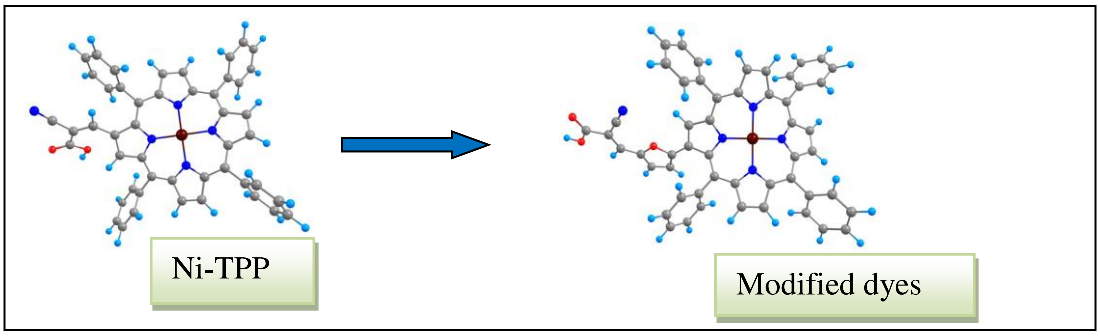

Figure 1: Modification of Ni-TPP CAA dye by introducing heterocyclic spacer

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E-140

Deep Dive into the Microstructures of Hybrid Electrolyte for K-ion Battery

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Due to the scarcity of Lithium, Potassium batteries are promising alternatives for large-scale energy storage devices, but they still require a lot of attention for their commercial survivability. For better performance of a battery, electrolytes play a crucial role. Previous studies mentioned that the formation of surface films near the electrode surface is mainly due to the decomposition reactions near the surface[1]. The solvation structure of cation in the electrolyte significantly controls the evolution of these films. So, in this work, we focus on the atomistic details of the bulk solvation structure of electrolyte solution [2]. Figure 1 shows the chemical structure of the salt and solvent used in this study.

We have performed classical molecular dynamics simulation at 298.15 K for three different electrolytes. The forcefield was validated by comparing the physical properties of the electrolytes with the experimental data. The preliminary idea of microstructures is obtained from the other structural analysis. The ion cluster analysis showed that different percentages of microstructures exist in the electrolyte. The energy levels that exist among the microstructures were calculated, and stability was studied.

Further, we implement various techniques to understand the dynamics of the active ion and the underlying mechanism of ionic transport. The mean square displacement and diffusivity obtained the dynamics. The heterogeneity in dynamics was obtained by calculating the Non-gaussian parameter [3]. The calculation of the self part of the van Hove function showed the diffusive motion of the ion.

Lastly, we calculated the lifetimes of different interactions in the electrolyte to understand the most and least-lived species. The insights obtained from this work will help researchers understand the interactions between different salt and solvent moieties that lead to different microstructures. This information will be advantageous for further developing electrolytes that could deliver better battery performance.

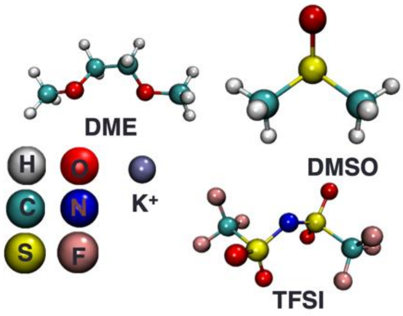

Figure 1 Chemical structures of different entities used in this study.

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E-141

Effect of Phosphorus doping on the hydrogen desorption temperature of MgH_2

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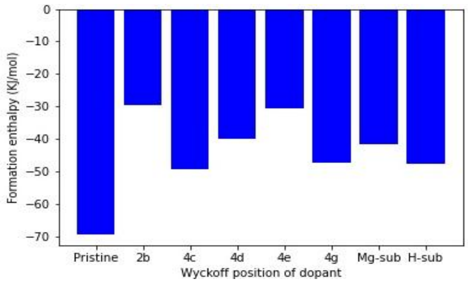
Hydrogen is an energy carrier that has potential to cater the future energy requirements. It is a potential alternative to fossil fuels. For its practical use, it has to be stored. There are different methods to store hydrogen. Among them MgH_2 is a good system to store hydrogen due to its good gravimetric and volumetric density, good reversibility, good abundance, non-toxic nature and low cost. But it suffers from slow kinetics and high desorption temperature [1]. Different methods are being explored to improve the kinetics and desorption temperature of MgH_2 system i.e. reducing particle size, doping with transition metals, metal oxides, chlorides etc [1]. In present study, we predict the effect of phosphorus on the desorption temperature of MgH_2 system using DFT (Vienna Ab initio Simulation Package). Crystal structure of MgH_2 is rutile (tetragonal, Space group No. 136, P42/mnm) [2]. K-mesh and energy cut off was optimized for Pristine MgH_2 and structure was relaxed. Lattice parameter was found a = b = 4.438 and c = 2.985 Å which is in well agreement with literature data [2]. 2×2×2 ($Mg_{16}H_{32}$) supercell was used for doped system. One P was doped at Mg substitutional, H substitutional, and interstitial doping sites. Different sites from 2a to 4g Wyckoff positions were selected for doping. K-mesh of 5×5×7 was used for Brillouin zone sampling. Structures were relaxed, and final calculations were done using tetrahedron method for better accuracy. Formation enthalpies were calculated for all MgH_2-P doped systems using equations (1-3). Formation enthalpies and desorption temperatures are given in Fig.1(a)&(b). 4c Wyckoff position is found the most favourable doping site for P.



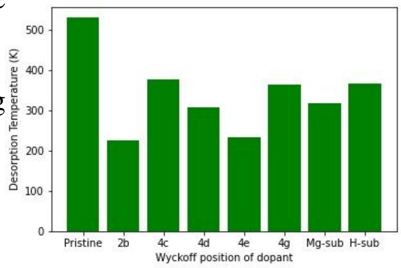


Figure 1(a). Formation enthalpy of pristine and P doped MgH_2 systems. Figure 1(b). Desorption temperature of pristine and P MgH_2 systems

$$\Delta H_{(Mg16DH32)} = 1/16\,(E_{tot}(Mg_{16}PH_{32}) - 16E(Mg) - E(P) - 16E(H_2)) \qquad (1)$$
$$\Delta H_{(Mg15DH32)} = 1/16\,(E_{tot}(Mg_{15}PH_{32}) - 15E(Mg) - E(P) - 16E(H_2)) \qquad (2)$$
$$\Delta H_{(Mg16DH31)} = 1/16\,(E_{tot}(Mg_{16}PH_{31}) - 16E(Mg) - E(P) - (31/2)E(H_2)) \qquad (3)$$

Where, ΔH = enthalpy of formation, E_{tot} = Total energy of system after doping, E(P) or $E(H_2)$= Ground state energy of P or H_2 in their standard states. Gravimetric density for pristine MgH_2 is 7.6% and after P doping reduce maximum to 7.08% which is well above the ultimate limit given by U. S. Department of Energy (6.5%). Bulk modulus was also calculated for all doped systems and systems were found mechanically stable and there is no much change in bulk modulus compare to pristine. Desorption temperature for pristine and most favoured P doped system (4c) was calculated and found 531 K and 377 K. In conclusion, P doping at low concentration (6.85 % by weight for interstitial doping) can improve the desorption temperature of MgH_2 system.

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E-142

Unlocking the potential of Na-rich cathode material through stabilizing oxygen redox using first-principles calculations

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In recent years, anionic redox chemistry has garnered significant attention for its application in the development of high-capacity battery materials. However, the incorporation of reversible anionic redox chemistry into cathode materials remains a challenge, primarily due to the release of gaseous molecular oxygen and resulting structural degradation upon cycling. In the present study, we systematically utilized the machine learning (ML) models and first-principles computational method (density functional theory, DFT) together to screen and elucidate the structural stability of pristine and doped Na-rich cathode material, Na_2RuO_3 at various deintercalation levels. We systematically investigate the electronic structure of a series of metal-doped Na_2RuO_3 compounds to demonstrate a strategy that how electronic structure tuning helps to adjust the extent of anionic redox in sodium-ion batteries (SIBs). Furthermore, we provide a systematic strategy for achieving reversible anionic redox and emphasize that it depends on multiple factors governing the electronic structure of the material, rather than solely relying on the covalent interaction between the transition metal and oxygen. Utilizing the aforementioned strategy, we identify a doped Na-rich material, capable of exhibiting reversible cationic and anionic redox. Additionally, we elucidate the reasons for the prevalence of cationic redox over anionic redox in pristine Na_2RuO_3. Our results not only advance fundamental knowledge but also offer valuable guidance for experimental endeavors aimed at enhancing existing materials and designing innovative cathode materials.

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E-143

Computational Study of Heteroatom-Doped Graphene Composite with Ru Metal Catalysts for Enhanced Li-S Battery Technology

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Lithium-sulfur (Li-S) batteries face several significant challenges that limit their practical use. To address these challenges, we design heteroatom (B, N, P, S, O) doped and metal-incorporated graphene as a catalyst, which improves electrical conductivity, provides active sites for polysulfide adsorption, and offers a robust structure that accommodates volume fluctuations. Our results, based on machine learning interatomic potentials (MLIPs) in conjunction with first-principles DFT calculations, show that the investigated systems offer better sulfur utilization, reduced capacity loss, and enhanced cycle life. Furthermore, we demonstrate that the catalytic properties of metal-doped graphene promote faster conversion of polysulfides, leading to improved reaction kinetics and overall battery efficiency. Specifically, incorporating Ru into heteroatom-doped graphene improves the electrical conductivity of the sulfur cathode, effectively mitigating inherent conductivity issues. This material further enhances its ability to bind polysulfides, reducing their dissolution into the electrolyte and minimizing the detrimental shuttle effect. Furthermore, Ru's catalytic properties can facilitate more efficient conversion reactions during charge and discharge cycles, improving capacity and cycle stability. Overall, Ru-based nitrogen-doped graphene provides a synergistic effect that enhances the electrochemical performance and longevity of Li-S batteries. we provide a computational protocol for pre-screening effective catalysts for Li-S batteries.

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E-144

Density Functional Theory Study of V@GaN as a Single-Atom Catalyst for CO_2 Reduction

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Anthropogenic carbon dioxide from industry and transportation significantly impacts the atmosphere, driving climate change and global warming. Carbon capture, conversion, and utilization offer promising solutions to reduce CO_2 emissions. Converting CO_2 into value-added fuels helps control global CO_2 levels and provides valuable fuels for various applications. The role of catalysts in the electrochemical CO_2 reduction reaction is crucial[1]. This work uses a first-principles method to investigate V@GaN (Fig.1a) as a catalyst for electrochemical CO_2 reduction [1]. The cohesive energy for V@GaN was found to be E_{coh}=-4.12 eV. Ab initio molecular dynamics (AIMD) simulations (Fig.1b) revealed the high thermal stability of the catalyst at T=300 K. According to the band structure, the catalyst exhibits a metallic nature. The two reaction pathways leading to intermediates, namely, formyl (OCHO) and carboxyl (COOH), are carried out [2]. A comparison of Gibb's free energy (ΔG) for the formation of primary intermediates of the CO_2RR (ΔG(*COOH) & ΔG(*OCHO)) and HER (ΔG(*H)) revealed that the catalyst shows selectivity toward the CO_2RR (Fig.1c) over the HER. The formation of *CO is the rate-determining step (RDS), with a limiting potential U_L=-0.69 eV. The calculated ΔG for the desorption of CH_3OH is -0.01 eV, whereas the ΔG for CO is 0.69 eV. This shows that V@GaN favors the formation of CH_3OH as a product with a lower overpotential of η=0.71 eV. In addition, V@GaN tends to suppress the HER and shows better catalytic activity towards CO_2 reduction with a lower overpotential.

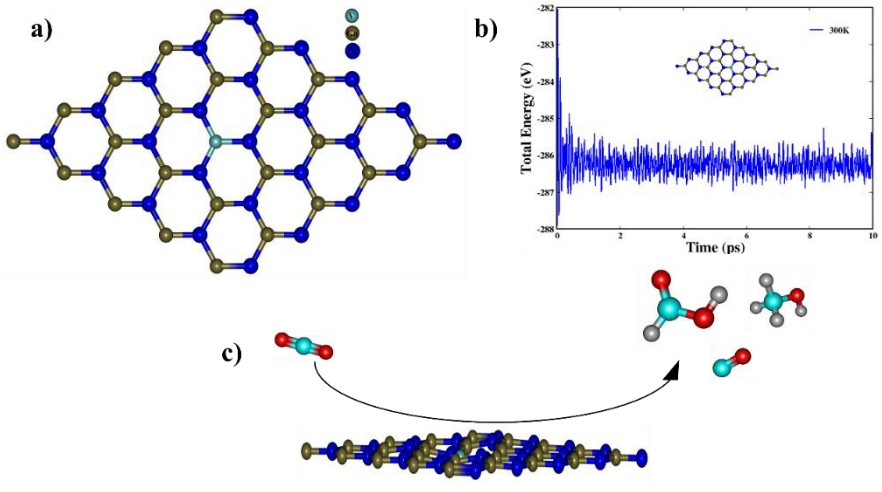

Figure 1. a) Optimized structure of V@GaN, b) AIMD of V@GaN at 300 K and c) CO_2RR occurring on V@GaN

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E-145

Understanding Electronic Properties of Prussian Blue Cathode Material for Potassium-ion Battery from First-principles

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Open frame network in Prussian blue analogues (PBAs) make them promising materials for their application as a solid electrolyte in large-scale energy storage [1]. Besides these materials are cost-effective and environmentally friendly. We have tried to establish a correlation between K+ conductivity, water content and ionic size of N-coordinated transition metal ions using the density functional theory calculations. The change in bandgap, lattice parameter and energy barrier during ionic diffusion process for these PBAs has been studied.

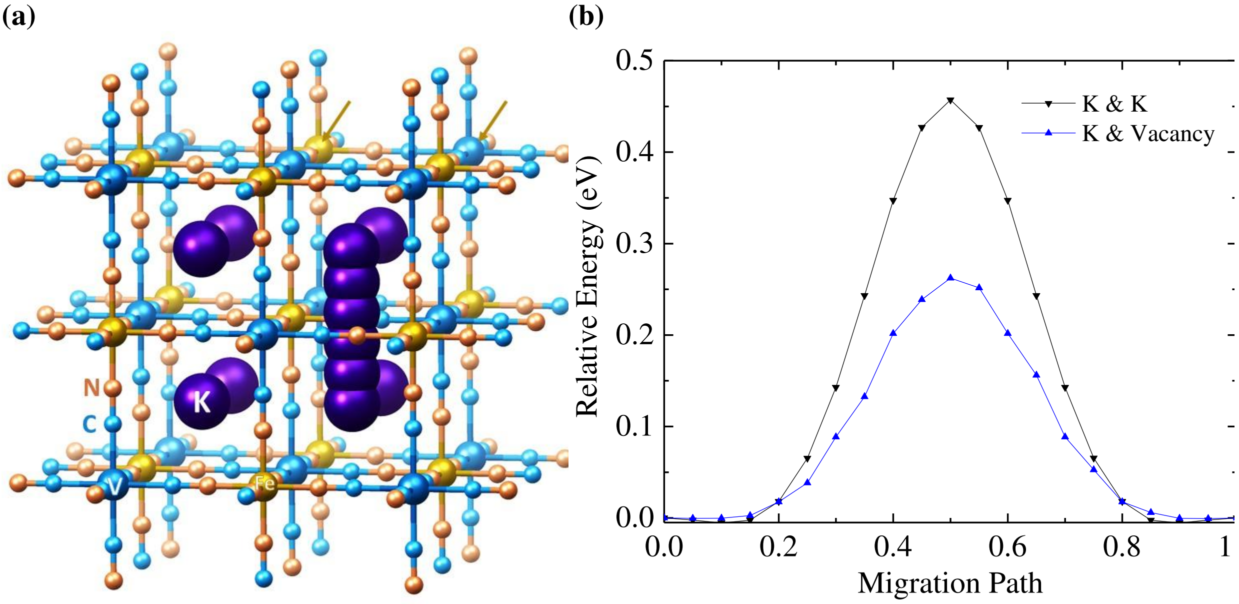

Figure 1. (a) Possible K+ diffusion pathway inside ideal Potassium Vanadium Hexacyanoferrate (VHCF) structure. (b) Energy barrier profiles of ionic diffusion in VHCF structure.

Figure 1 shows the possible diffusion pathway (a) and the corresponding energy barrier for Potassium Vanadium Hexacyanoferrate (K-VHCF). It is evident that the energy barrier of the K-VHCF with K vacancy at one site (¾, ¾, ¾) is significantly lower than the one with fully occupied K sites. Our study provides an insight into the designing of advanced electrolyte material based on open architecture PBAs for improved battery performance.

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E-146

Capture and Complexation of Carbon Monoxide Using NHC and NHC Boryl anion Ligands: A Computational Study

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Carbon monoxide (CO) is a highly toxic pollutant with significant environmental and health risks, resulting from the incomplete combustion of carbon-containing fuels. Addressing CO emissions is critical, and various methods have been developed to capture and eliminate this gas. Among these, N-Heterocyclic Carbenes (NHCs) have gained attention due to their unique electronic properties, including high donating ability and exceptional stability, enabling them to form strong complexes with various elements[1]. Recent research has highlighted NHC's potential in stabilization applications, particularly in stabilizing complexes of the general form L-E-E-L, where E represents elements like Si[2], Ge[3], P[4], and As[5], and L is an NHC ligand. A recent report has demonstrated the capture of carbon dioxide by bis(N-heterocyclic carbene)-borylene complexes, facilitated by the low π-acidity of NHC, which maintains the nucleophilic properties of borylenes[6].

This study explores the interaction between CO and NHC ligands, along with their boron analogs, specifically N-Heterocyclic carbene boryl anions, in the form L-CO-L, highlighting its potential for future applications in CO capture. A density functional theory (DFT) approach was employed, using the M06-2X functional with the 6-311++G(d) basis set, to optimize the geometries and analyze the electronic stability of the formed complexes. The study was extended by placing both electron-donating and electron-withdrawing substituents on the NHC ring. It was observed that the configuration with an electron-donating group on the oxygen side of CO and an electron-withdrawing group on the carbon side yielded the most stable complexes.

The findings indicate that while NHC ligands can form CO complexes with relatively low stabilization energy, the boron analogs offer a more robust and stable approach to CO capture. This study contributes to the growing body of research on main group chemistry and the development of novel methods for CO capture, which is essential for mitigating its environmental impact.

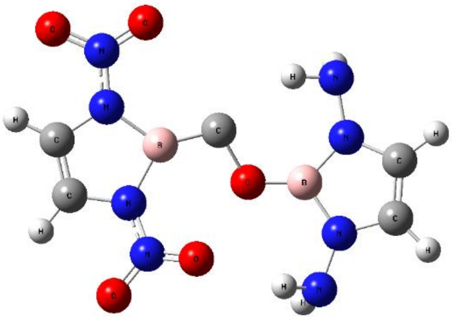

Figure 1. Computed structure of the most favourable $[(C_2H_2BN_2(NH_2)_2)(C_2H_2BN_2(NO_2)_2)CO]^{-2}$ complex

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E-147

Spin Engineering of Tetracoordinated Boron Doped TG[3] Systems and its Nonlinear Optical Properties

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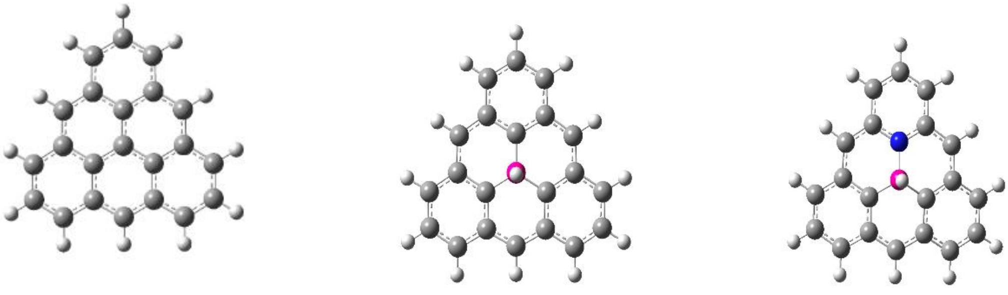
Organic nonlinear optical (NLO) materials are garnering considerable interest due to their exceptional optical and electronic characteristics. Recently, the spin engineering of nanographenes (NGs) has received significant attention for their potential applications in next-generation optoelectronic and NLO materials. Among these, triangulenes, a class of open-shell NGs, have emerged as particularly promising due to their unique spin properties [1]. The electronic and magnetic properties of triangulenes can be further tailored through heteroatom substitution, such as doping with boron and other elements. This modification provides additional opportunities to modulate their properties, enhancing their value for applications in organic electronics. Boron is particularly notable for its versatile chemistry across various compounds, and the tetracoordinate boron has gained significant attention due to its distinctive electronic properties [2]. Furthermore, doping with heteroatoms like nitrogen can alter the spin multiplicity of the system, which in turn can influence its NLO properties [3]. This study investigates the nonlinear optical (NLO) properties of tetra-coordinated boron-doped TG[3] systems, focusing on both peripheral and central doping effects. Spin engineering is applied to further enhance and understand the NLO behaviour, with the aim of optimizing these systems for advanced optoelectronic applications. Preliminary results indicate a significant impact of spin configuration on the hyperpolarizability of the complex, suggesting its suitability for advanced optoelectronic applications. All calculations were performed using the DFT/B3LYP method with the 6-31+G(d,p) basis set, utilizing the Gaussian 09 program. Further exploration is underway to optimize these properties and to understand the underlying mechanisms driving the observed NLO behaviour.



(a)**TG[3]** (b) **B-H TG[3]** (c) **1N B-H TG[3]**

Figure 1. Optimized geometries of (a) tringulene TG[3], (b) tetracoordinated boron doped triangulene B-H TG[3], and (c) one nitrogen doped tetracoordinated boron doped triangulene 1N B-H TG[3].

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E-148

Adsorption and Dehydrogenation of Ammonia on Ru@Cu(111) Surface: A DFT Study

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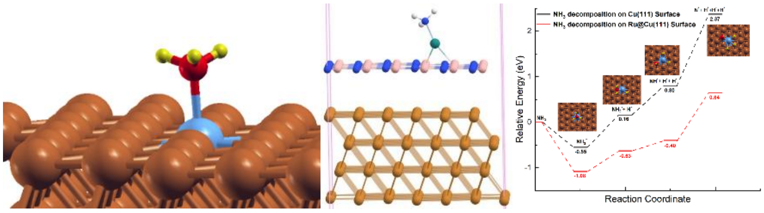
The catalytic performance and surface chemistry of NH_3 decomposition has become very important to understand for molecular hydrogen generation. Ru has been regarded as a very good catalyst for ammonia (NH_3) decomposition as Ru lies in the optimum position of the volcano curve which depicts the choice of materials for NH_3 decomposition [1]. The adsorption and successive dehydrogenation mechanism of NH_3 on Cu(111) and Ru@Cu(111) surfaces have been systematically investigated by using density functional theory (DFT) method with a periodic slab model. All the possible adsorption configurations of relevant intermediates on Ru@Cu(111) and Cu(111) surfaces are identified. The adsorption energies of NH_x(x=0-3) species exhibit the following trend: NH_3<NH<NH_2<N for Ru@Cu(111) surface and NH_3<N<NH<NH_2 for Cu(111) surface depending on the site of their stability. The successive dehydrogenation path of NH_3 into adsorbed N and H-atom is identified to explore the dehydrogenation mechanisms on different surfaces. The total reaction energy of NH_3 decomposition has been reduced from 2.54 to 0.75 eV and that associated with the last step of NH dissociation has also reduced from 1.37 to 0.15 eV, while substituting a Cu atom with Ru. It implies that the complete dehydrogenation of NH_3 on Ru@Cu(111) surface is thermodynamically favourable and the doped Ru atom in the top layer acts as the reaction active centre. It is also found that the reaction energy associated with the associative desorption of N_2 molecule gets reduced when a Cu-atom in Cu(111) surface is substituted by a Ru-atom, and that will help in the regeneration of catalyst. From the elemental structure calculation, it is found that the calculated adsorption and activation energies mainly depend on the *d*-band centre of the metal surface under study. The successive dehydrogenation of NH_3 on Ru adatom *h*-BN sheet supported on Cu surface *i.e.* Ru@BN-Cu(111) has also been investigated. The barrierless H_2 molecule release from two adsorbed H atoms on Ru@BN-Cu(111) surface makes it a better catalyst compared to Ru@Cu(111) surface.



(a) (b) (c)

Figure 1. (a) NH_3 adsorbed on top of Ru@Cu(111) surface; Atomic symbols: Sky Blue ball=Ru, Brown ball=Cu, Red ball=N and Yellow ball = H. (b) NH_3 adsorbed on Ru@BN-Cu(111) surface Atomic symbols: Green ball=Ru, Brown ball=Cu, Blue ball=N and White ball = H. and (b) Thermochemistry of NH_3 decomposition on Ru@Cu(111) and Cu(111) surfaces.

Table 1. Adsorption energy E_{ads} (eV), M-N bond length d_{M-N} (Å), (M=Ru, Cu), N-H bond length d_{N-H} (Å) and H-N-H bond angle <H-N-H (in degree) for NH_3 adsorbed (at top site t1) Ru@Cu(111) and Cu(111) surfaces.

Species(s)	E_{ads}	d_{M-N}	d_{N-H}	<H-N-H
Ru@Cu(111)-NH_3	-1.08	2.20	1.02	108.4
Cu(111)-NH_3	-0.55	2.11	1.02	107.7

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E-149

Screening of Anion in Ionic Liquid - Graphene Interface for the Energy Storage Applications: First Principles Approach

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Graphene is a 2D material which is widely used in energy harvesting application, also it is well known for its zero band gap. Along with graphene, ionic liquids (ILs) are widely used as electrolytes due to the excellent ionic conductivity and stable electrochemical window.[1,2] Here, we made an effort to analyze the changes in electronic structure of graphene with various adsorbed ILs (collectively called as GRAPHIL). In this study, we have taken series of ILs with hydrophobic/hydrophilic anions and common MMIm cation.[3,4,5] To get more insights on the complex structure, stability, selection of a suitable density functional theory (DFT) method is important to study the interfacial influence of IL at the graphene surface. Here, the interaction of ILs such as $[MMIm]^+ [X]^-$ (where, X=OAc, $AlCl_4$, PF_6, BF_4, Cl, OTf, Tf_2N and DCA) with graphene is studied. We found that the physisorption mechanism of ILs on the graphene surface is mainly driven by the anions through different mode of interaction. Furthermore, energy-minimized structure, adsorption energy, projected density of states, band structure and charge transfer indicates that the interaction between GRAPHIL is dominated by non-covalent forces. Interestingly, the electronic and quasi-metallic behavior are governed by tuning of anion of ILs. Our findings reveals that, chemical composition of elements and size of the anions plays the vital roles in strength of interaction between the GRAPHIL. Our study can provide valuable microscopic-level information to predict potential supercapacitor materials for energy storage applications.

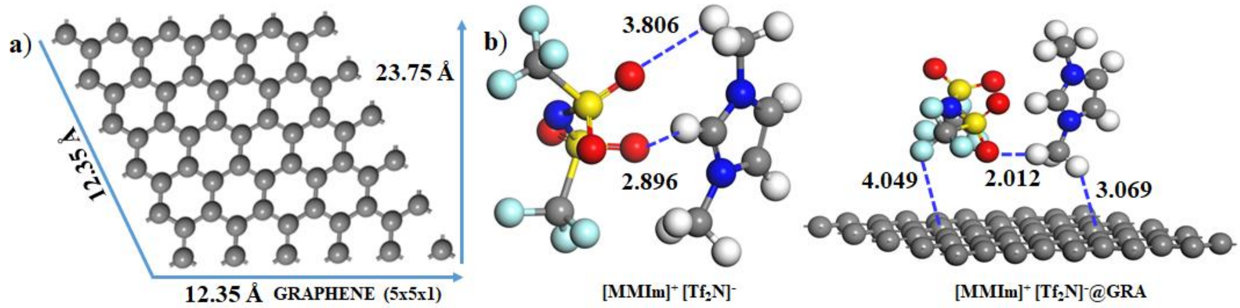

Figure .1 a) Mono layer of graphene surface (5x5x1). b) Energy minimized geometry of $[MMIm]^+[Tf_2N]^-$ and $[MMIm]^+[Tf_2N]^-$ @Graphene

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E-150

Understanding the Structural Properties of Polybenzimidazoles In Water Salt Mixtures using Atomistic Molecular Dynamics Simulations

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Polybenzimidazoles (PBI) are the class of charged polymers with charged benzimidazole moieties as their structural repeat unit. Depending on their charge, PBIs are called cationic or anionic ionone's, and they have excellent thermo-mechanical characteristics. The PBI has been extensively used as electrolyte systems[1], a variety of difficult gas and liquid separations, etc.[2] However, molecular understanding of the structural properties of PBI is intriguing.

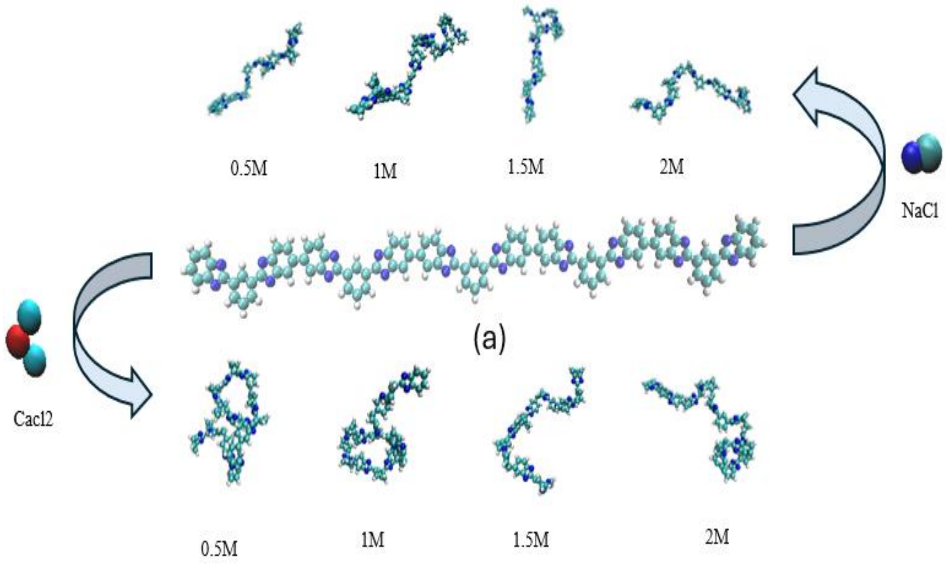

Figure 1. The initial and final structure of PBI after MD in salt-water systems.

In this work, we performed atomistic molecular dynamics(MD) simulations to understand the structural properties of PBI in the saltwater mixture. Two different salts are considered sodium chloride (NaCl) and calcium chloride ($CaCl_2$). We present various inter and intra-molecular structural properties such as radius of gyration, intermolecular and inter-atomic radial distribution functions, hydrogen bonding analysis, and dihedral angle analysis. Our results show a decrease in the radius of gyration(R_g) of PBI with an increase in salt concentration from 0 M to 2 M for both salts. We observe a 22% decrease in R_g in $CaCl_2$ and 7% in NaCl.

We see significant PBI chain coiling in $CaCl_2$ salt when compared to NaCl salt as shown in Figure 1. Furthermore, we also observe a number of hydrogen bonds show a 45% decrease for $CaCl_2$ due to strong intra-molecular interactions. Radial distribution function(RDFs) results, dihedral distribution, and solvent accessible surface area(SASA) are in accordance with the R_g and H-bond. Overall, the results presented in this work will give an understanding of complex interactions between PBI and monovalent and divalent salts (NaCl and Cacl2) with water as a solvent.

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E-151

Design of Different Water Channel Morphologies in Hydrated PEM using Molecular Modelling and Simulation Approach

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Proton Exchange Membranes (PEM) are ion-exchange membranes used in various applications, including fuel cells, electrolysers, mobile devices, and power units. The effectiveness of PEMs depends on the degree of hydration (λ), which is the ratio of hydronium ions and water molecules to fixed counter-ions [1]. The transfer of proton through PEMs depends on the morphology of the hydrated channels in the membrane. The Grotthuss mechanism transfers proton through the PEM based on hydrogen bonds with water molecules, while the vehicular mechanism transfers proton via diffusion. PEMs are widely used in Direct Methanol Fuel Cells (DMFCs) due to their simplicity, high energy density, and ease of refueling.

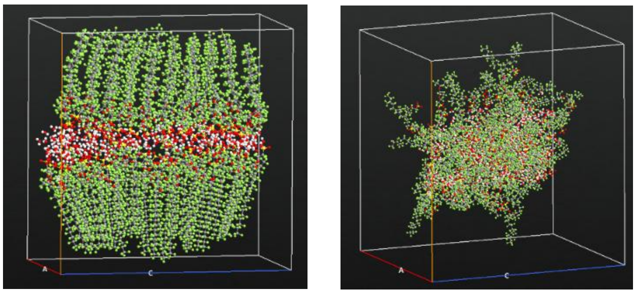

Figure 1. Structures of hydrated Nafion with λ = 3. (a)Lamellar (b)Random

Table 1. Properties of structures

Structures	Hydration degree	Total no of atoms
Random	3	$C_{1782}F_{3525}H_{567}O_{648}S_{81}$ (6603 atoms)
	6	$C_{1782}F_{3525}H_{1053}O_{891}S_{81}$ (7332 atoms)
	9	$C_{1458}F_{2877}H_{1539}O_{1134}S_{81}$ (7089 atoms)
Lamellar	3	$C_{1782}F_{3645}H_{567}O_{648}S_{81}$ (6723 atoms)
	6	$C_{1782}F_{3645}H_{1053}O_{891}S_{81}$ (7452 atoms)
	9	$C_{1458}F_{2961}H_{1539}O_{1134}S_{81}$ (7173 atoms)

The molecular structure of hydrated Nafion membrane with random and lamellar water channels has been developed and optimized using Quantum ATK® software. The structure closely aligns with literature, and the morphology of the water channel determines the effective interaction of the PEM with the water-hydronium mixture [2]. Further work is being performed to characterize hydrated PEMs for varying degrees of hydration and quantify methanol crossover through these membranes. This understanding will help design better PEMs for DMFCs with lesser methanol crossover without affecting proton conductivity.

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E-152

Designing Improved Catalysts for Oxygen Evolution Reaction by Harnessing Lithium Electrochemical Tuning using Density Functional Theory Calculations

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Finding effective catalysts for water splitting and Oxygen Evolution Reaction (OER) is important for enhancing the efficiency of energy conversion and storage technologies. Platinum is a highly efficient catalyst for OER but due to its high cost and scarcity, platinum is not ideal for large-scale applications. Lithium metal oxides have gained significant attention in recent years for their application in electrocatalysis for OER. The electrochemically tuned $LiCoO_2$ for oxygen evolution reaction and increase in catalytic activity upon electrochemical deintercalation was already studied using both experimental and computational methods [1] But $LiCoO_2$ are very expensive due to the cost of cobalt. To address this drawback, in this study we have investigated the change in electronic structure of other Lithium metal oxides like $LiNiO_2$ and $LiMnO_2$ upon deintercalation by employing DFT computational methods. Further, we systematically investigate the nickel and manganese doped $LiCoO_2$ and the effects attributed by change in oxidation states of metals and its strong covalent coupling to the 2p states of oxygen. Our study aims to design a rational and cost-effective catalyst for large scale industrial OER.

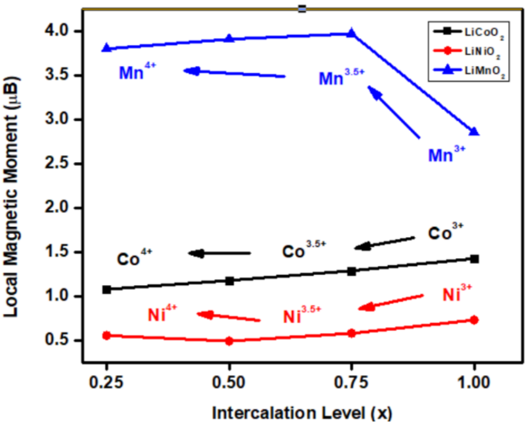

Figure1.Schematic representation of local magnetic moment of $LiCoO_2$, $LiNiO_2$,and $LiMnO_2$.

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E-153

Phenothiazine Derivatives For Efficient Organic Dye-Sensitized Solar Cells

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Dye sensitized solar cells (DSSCs) are becoming the field of interest for many researchers due to their cost-effectiveness, versatility and environmentally friendly technology. In 1991, the DSSC concept was first invented by Brian O'Regan and Michael Gratzel using mesoporous TiO_2 nanoparticles and ruthenium dye, and best photoconversion efficiency of DSSC is 14.3%. Commonly, Ru-polypyridine complexes, dyes are widely used and showed efficiencies of up to 11%.[1] But due to their high cost and requires careful synthesis we are go towards metal-free organic dyes.

Metal-free organic dyes are inexpensively, simpler molecular design and environment friendly and they offer the possibility of low-cost conversion of photovoltaic energy. The major advantages of these metal-free dyes are their tunable absorption and electrochemical properties. Therefore, we recognized the significance of metal free organic dyes in DSSCs, we have chosen metal free organic dye i.e. PTZ (phenothiazine) derivatives for efficient organic dye sensitized solar cells. These dye synthesized easily with low cost materials which express higher efficacy for DSSCs. In this dye derivative, PTZ unit is adopted as an electron donor, thiophene group attached to the cyanoacrylic acid as the electron acceptors (anchoring groups), and butyl carbon chains to enhance solubility. In this theoretical calculation used CH_2Cl_2 solvent because we have found that it shows ideal g value. Density functional theory (DFT) calculations are performing at a B3LYP/6-31+G(d) level for the geometry optimization in order to get a further insight into the significant variations in performance of DSSCs based on these PTZ dyes.The frontier MOs of thiophene group attached to the cyanoacrylic acid reveal that HOMO–LUMO excitation move towards the electron density distribution from the PTZ moiety to the thiophene group attached to the cyanoacrylic acid moiety. However, the LUMO electron density geometry distribution of PTZ derivative is located on the thiophene cyanoacrylic group. Consequently, the PTZ derivative effectively injected electrons into the TiO_2 conduction band. These results indicate that the PTZ derivative dye can give fast electron injection from the LUMO to TiO_2. We have showed that the LUMO of PTZ derivative dye has better orbital overlap with the TiO_2 conduction band. [2]

In conclusion, we have synthesized a novel series of PTZ derivative dyes for DSSCs. A noticeable solar energy-to-electricity conversion efficiency (g) of 5.5% is achieved in a DSSC based on PTZ derivative dye, which is simple in structure and easy to synthesize. For this purpose, we have studied the structural, electronic and optical properties of PTZ (phenothiazine) derivative dyes in CH_2Cl_2 solution, using first principles density functional theory (DFT) and time dependent density functional theory (TDDFT), with the objective of moving towards a class of better sensitizers for dye sensitized solar cells (DSSCs). Absorption and emission spectra are measured in CH_2Cl_2 solution (2×10^{25} M) at room temperature. DFT is used to determine the structural and electronic properties of the dye. TDDFT is used to determine the optical properties and absorption spectra. Detailed natural transition orbital (NTO) analysed offer vital insight into the relevant charge transfer mechanisms. The structural modifications attempted here are found to lead to improved light harvesting efficiencies (LHE). The geometrical index (t_4) is used to confirms a distorted tetrahedral ground state geometry for a PTZ dye derivative solar cell. The electronic projected density of states (PDOS) is calculated using a double-zeta-valence polarized (DZVP) basis set. The highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) of dye are also determined from the PDOS. Therefore we have found that the LUMO of PTZ derivative dye has better orbital overlap with the TiO_2 conduction band and simple in structure and easy to synthesize.

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E-154

Modeling of Solid-Oxide Fuel Cells

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Solid Oxide Fuel Cells (SOFCs) are advanced electrochemical devices that convert chemical energy directly into electrical energy with high efficiency and low environmental impact. The performance and durability of SOFCs are heavily influenced by the materials used in their construction, particularly the effects of various dopants on their structural, electrical, and catalytic properties. The choice of materials for SOFC design, including electrolytes, anodes, cathodes, and interconnects, is crucial for optimizing performance.

Materials such as yttria-stabilized zirconia (YSZ), gadolinium-doped ceria (GDC), and lanthanum strontium manganite (LSM) are commonly used due to their favorable properties. The poster will explain the key factors influencing SOFC design, including the effects of dopants, reactivity on different planes, and the selection of suitable materials, aiming to provide insights into enhancing the efficiency and applicability of SOFC technology.

Keywords: nudged elastic band, adsorption energy, density of states, band structure, energy efficiency

F-121

Photoexcited Charge Carriers Dynamics in Fullerenes Encapsulated by Covalent Organic Polyhedra: Choice of Fullerene Matters

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Charge separation is in the heart of solar energy applications, and efficient materials require fast photoinduced electron transfer (ET) and slow electron-hole (e-h) recombination. Employing time-dependent self-consistent-charge density functional tight-binding theory combined with nonadiabatic molecular dynamics [1], we report a detailed analysis of ET and e-h recombination in hybrids composed of photoactive covalent organic polyhedra (COP) and encapsulated fullerenes and optimized geometry of COP@C70 is shown in Figure 1a. The ET occurs on ultrafast timescale, and accelerates with increasing fullerene diameter, C_{60} to C_{70} to C_{84}, see Figure 1b. As the fullerene size increases, the π-electron system available for interaction with the COP grows, the fullerene-COP separation decreases, and the number of fullerene states available to accept the photoexcited electron increases, accelerating the ET. In comparison, the e-h recombination occurs on a nanosecond timescale (Figure 1c) and correlates with the length of the fullerene shortest axis, because the relevant fullerene state is polarized in that direction. The largest and least symmetrical C_{84} exhibits the fastest ET and the slowest e-h recombination, making COP@C_{84} the most promising hybrid. Both high-frequency bond stretching and bending vibrations, and low-frequency breathing modes are involved in the ET and e-h recombination processes, with more modes present in the C_{84} system due its lower symmetry. The 10-20 fs vibrationally induced quantum coherence loss in the electronic subsystem contributes to long lifetimes of the charge-separated states. The comprehensive investigation of the structure-property relationship of the charge carrier dynamics in the COP@fullerene hybrids provides a detailed atomistic understanding of interfacial ET processes and generates guidelines for rational design of high-performance materials for solar energy and related applications.

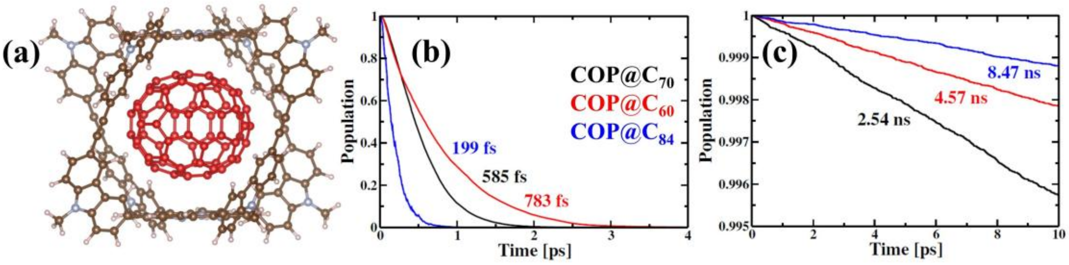

Figure 1. (a) Optimized geometry of COP@C70 nano hybrid. Decay of population of the donor states for (b) electron transfer and (c) charge recombination in COP@C70 (black), COP@C60 (red) and COP@C84 (blue).

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F-122

Importance of Polarizable Force Fields in MD Simulations: A case study of the effect of higher chalcogen substitution in the amide group on the self-assembly of benzene-1,3,5-tricarboxamide

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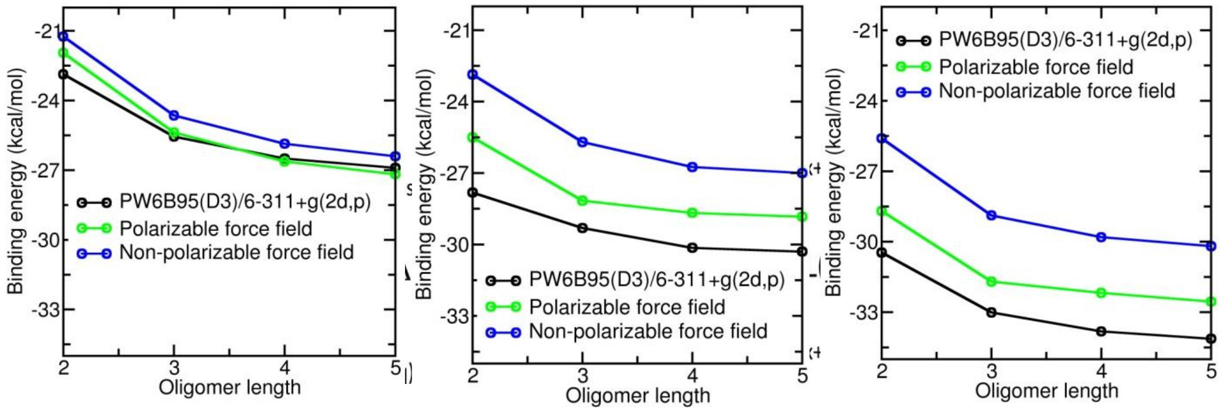
For a long time, experimental [1] and computational efforts have concentrated on alkyl-substituted C=O centered benzene-1,3,5-tricarboxamides (OBTA) in the context of supramolecular polymerization, yielding in a comprehensive understanding of this system. Recently, inspired by the structural and catalytic changes observed with thioamide and selenoamide groups in proteins, researchers have begun exploring the replacement of the amide group in BTA with thioamide (SBTA) [1] and selenoamide (SeBTA) [2]. Experimental results indicate that oligomers exhibit thermal stability in the order SeBTA > SBTA > OBTA, while their cooperativity in supramolecular growth follows OBTA > SeBTA > SBTA. These differences are attributed to increased polarizability and changes in electronic properties.

While OBTA polymerization has been extensively studied using MD simulations, those of SBTA and SeBTA have not. Quantum chemical calculations indicate that sulfur and selenium substitution enhancedispersion interactions, polarizability, and charge transfer, underscoring the need for polarizable force fields for accurate modelling. We thereby employed the Drude oscillator model [3], which is known for its simplicity and computational efficiency as compared to other polarizable models, to dynamically adjust atom polarization.Using this model, our preliminary calculations comparing gas-phase binding energies of oligomers of varying sizes (Figure 1) showed that the results from polarizable force field aligns better with DFT calculations than those from the non-polarizable model. Inspired by these results, we aim to investigate these systems in explicit solvent to gain a deeper understanding of the microscopic interactions in supramolecular polymers.



(a) (b) (c)

Figure1: Binding energies of oligomers calculated using the Drude force field show improved agreement for (a) OBTA, (b) SBTA, and (c) SeBTA, with its significance being particularly evident for SBTA and SeBTA

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F-124

Solvation Behavior of Ions in Aqueous Taurine Mixtures and Counteraction Effects of Taurine on Urea-Induced Denaturation

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The solvation scenario of monovalent cations, anions, and molecular ions is explored in the binary mixtures of aqueous taurine and ternary aqueous urea-taurine solutions. [1-3] These studies are conducted at 308 K using classical molecular dynamics (MD) simulations up to 5 ns. We have also investigated the hydrogen bond dynamics between water–water, water–taurine, and ion–water/taurine interactions. Our results showed that monovalent cations have a higher affinity for the oxygen atoms of taurine, while anions interact with the hydrogen sites of taurine. Additionally, ammonium ion prefers the sulfonate oxygen of taurine. In contrast, acetate ions tend to interact more with the amino hydrogens of taurine than with the oxygen and hydrogen atoms of water. The hydrogen bond interactions between water and taurine were also analyzed through their respective radial distribution functions (RDFs), as shown in Figure 1. It was observed that taurine tends to donate hydrogen atoms to water molecules more than to accept hydrogen atoms from water. In both binary and ternary mixtures, the translational dynamics and orientational relaxation of the dipole vector of water molecules were found to slow down due to the formation of strong hydrogen bonds with taurine. The average lifetime of the water–water hydrogen bond ($O_W \ldots H_W$) was higher in the ternary mixture compared to the binary aqueous taurine solution. To further understand the effect of taurine in the presence of urea, MD simulations of 100 ns were conducted on human islet amyloid polypeptide (hIAPP) by varying the concentrations of urea and taurine in GROMACS 2020.1. [4] The findings indicate that taurine counteracts the urea-induced denaturation of hIAPP by restoring the secondary structure content at 5.6 M urea and 0.45 M taurine.

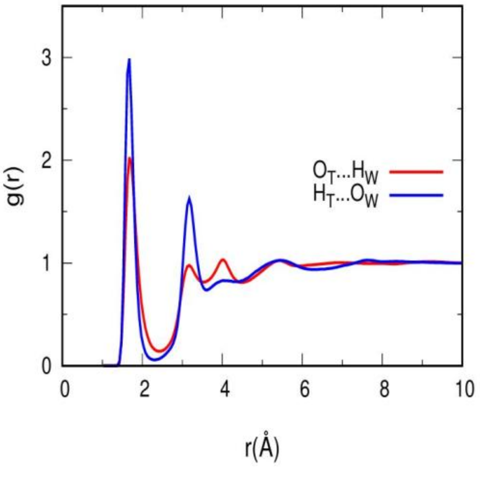

Figure 1: Radial Distribution Functions of $O_T \ldots H_W$ (red) and $H_T \ldots O_W$ (blue) in the aqueous solutions of taurine.

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Nanoscale Self-Assembly and Water Retention Properties of Silk- Riboflavin Hydrogel

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Silk-fibroin hydrogels have gained considerable attention in recent years for their versatile biomedical applications. The physical properties of a complex hydrogel, com- prising silk fibroin and riboflavin, surpass those of the silk-hydrogel without additives. This study investigates silk-riboflavin (silk-RIB) hydrogel at the atomistic level to uncover molecular structures and chemical characteristics specific to silk and riboflavin molecules in an aqueous medium.

The interplay between hydrophilic riboflavin and hydrophobic silk polymers facilitates the formation of solubilised silk fibre, which subsequently evolves into a nano-scale hydrogel over time. Eventually, the interlinked RIB stacks form a scaffold that not only accommodates silk aggregates but also encloses water pockets, preserving moisture levels and enhancing thermal conductivity of the hydrogel. To explore water retention properties and the role of ions, two sets of simulations of semi-hydrated hydrogel in the presence and absence of ions are conducted. The presence of ions significantly influences the dynamics of RIB and silk. Favorable interactions with the ions impede the unrestricted diffusion of these larger molecules, potentially leading to a stable structure capable of retaining water for prolonged duration. The complete removal of water results in further shrinkage of the anhydrous silk-RIB hydrogel or xerogel, yet its porosity and structural integrity remain intact. These findings offer valuable insights into the behavior of silk hydrogel and xerogel, paving the way for materials engineering in aqueous environments to develop biomedical devices with customized functional properties.

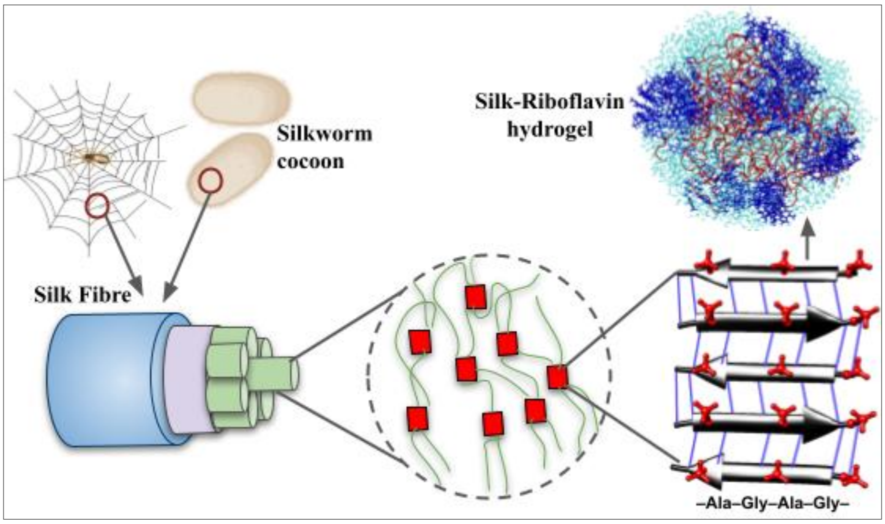

Figure 1. Overview of workflow

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Predicting Electrophoretic Mobility of Charged Particles in Aqueous Medium

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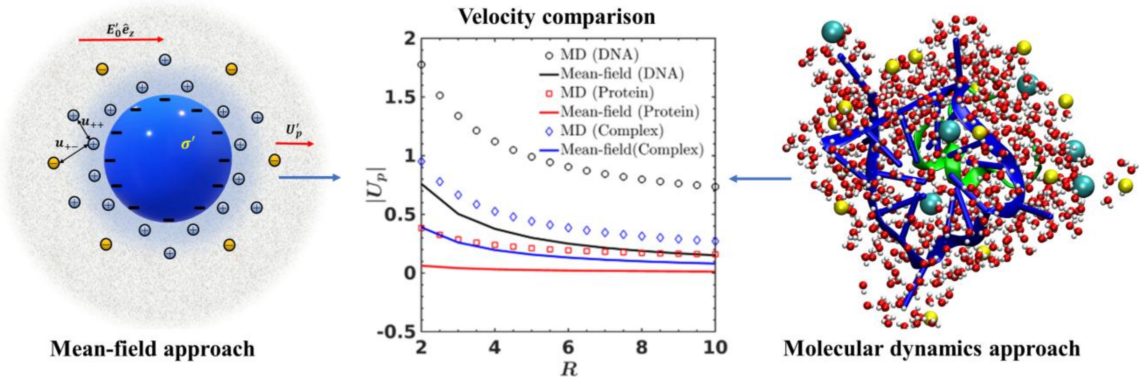
Electrophoresis of charged particles has important applications in biochemical separation processes. The mobility of these particles depends on the surrounding electric double layer (EDL), which is impacted by solvent restructuring because of hydration interactions. Nevertheless, most theoretical estimates ignore such interactions while computing the electrophoretic mobility. Here, we employ a complementary blend of mean-field analysis and MD simulations performed for a peptide-G-quadruplex complex to assess how hydration interactions alter the mobility of a charged particle in an aqueous medium [1]. These interactions are seen to stabilize the EDL, resulting in more significant localized counterion concentrations, whilst also strengthening the ensuing electrokinetic flow. The ordering of ions near the particle surface is only obtained upon including hydration interaction, revealing that the hydration water molecules act as a glue for forming a stable EDL, a key finding of this work. Conversely, the observed microstructure of ions near the charged surface as obtained from our theory establishes a bridge link between the micro and continuum model. The presence of larger counter ions enhances the drag on the particle, thus restricting its mobility. The mobility also becomes size-dependent, which may be useful for isolating a wide array of biomolecules. The impact of hydration interactions intensifies with increasing particle size, surface charge density, and bulk ionic concentration. Figure (1) depicts the schematic diagram for mean-filed and MD analysis in panel (a) and (c). In panel (b) we present the comparison of particle velocity magnitude obtained from the two approaches.



(a) (b) (c)

Figure 1. Panel (a) and (c) depicts the mean-field and molecular dynamic systems under consideration. Panel (b) represents the comparison of obtained velocity from both the methods.

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F-127

Constructing One-dimensional Supramolecular Polymer Structures Using Particle Swarm Optimization Technique

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Predictive accuracy of the properties of supramolecular polymers relies heavily on choosing good initial structure[1]. However, generating appropriate initial structures poses a significant challenge, primarily owing to the extensive range of potential configurations. To address this issue, we present StackGen, an open-source user-friendly framework designed to efficiently generate energy-optimized one-dimensional supramolecular polymer structures with minimal computational overhead.[3] StackGen leverages the efficacy of particle swarm optimization (PSO) algorithm in locating the global minimum structure for both simple and intricate molecules[2] in combination with a semiempirical quantum mechanical approach to identify low-energy supramolecular stackconfigurations from a diverse set of potential configurations. These configurations arise from the translational and rotational adjustments of adjacent molecules around monomers along various axes. This tool accounts for various structural factors, including the presence of functional side groups and the degree of intermolecular π-π stacking interactions. Our extensive testing of StackGen on different molecules varying in π -core and side-chain composition demonstrates StackGen's effectiveness and versatility to produce low-energy structures with negligible computational costs. Furthermore, this tool features real-time optimization of PSO hyperparameters, enhancing convergence. StackGen offers a convenient solution for generating supramolecular polymer structures suitable for both molecular simulations and quantum mechanical calculations, all within a user-controlled environment and with negligible computational cost.

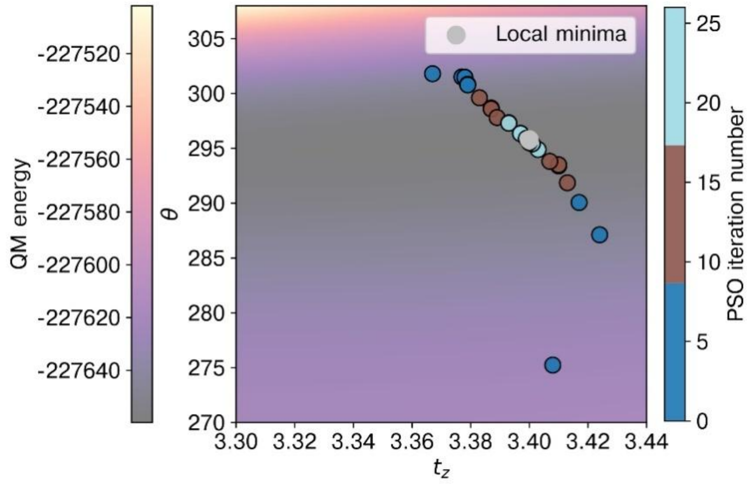

Figure 1. Scatter plot illustrating the progress of the optimal solution discovered by the swarm during each iteration of PSO

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F-128

Effects of Phytosterols' Chemical Composition on Membrane Biophysical Properties: Insights from MD Simulations

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Phytosterols are the plant derived sterols which have cholesterol-like structure and properties responsible for their large pharmaceutical and nutraceutical applications. They are the bioactive compounds having plethora of health benefits including anticancer, anti-inflammatory, anti-oxidant properties etc. Phytosterol are reported to have effective cholesterol lowering activity upon dietary intervention, leading to cut down the risks of cardiovascular diseases. As the integral membrane component, their mechanism of action mainly depends on their membrane modulation properties, which is attributed to their structural parameters. Therefore the impact of their small structural changes (Figure 1) on biophysical and physico-chemical characteristics of lipid membrane is crucial to elucidate.

In our study we have illustrated the structural and dynamical properties of two most abundant phytosterols i.e. β-sitosterol and stigmasterol, along with cholesterol, in simple model membranes consisting of DOPC/DPPC using all-atom molecular dynamics (MD) simulations. Both the sterols have shown cholesterol-like condensation effects but their extents differ with respect to their structural modifications. We observed cholesterol showing large-scale phase separation, with the co-existing ordered and disordered domain in line with previous reports. However incorporation of additional ethyl group in alkyl tail of other two sterols, exerts subtle changes in lipid ordering but, affects lipid packing and miscibility considerably. Maximum impact observed in the case of stigmasterol with additional unsaturation, which prevents the large-scale phase separation, resulting in the formation of small domains. Such behavior could have large impact on the formation of functional nanodomains in the membrane. Therefore the relevance of this work lies in the comprehensive understanding of phytosterol/lipid interaction via in-silico approach at their atomistic level to establish the structure-function relationship of phytosterol aid to their potential applications.

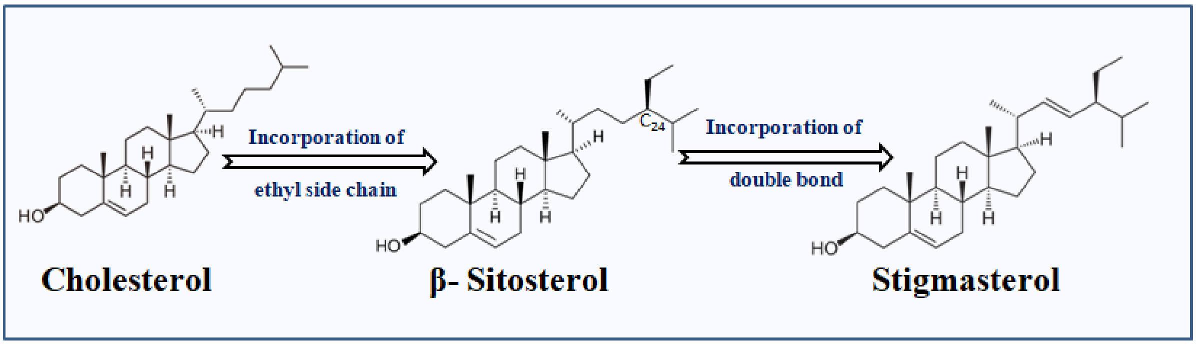

Figure 1: Chemical Composition of Stigmasterol and β-Sitosterol

G-121

Vibronic Coupling in First Five Electronic States of P_2N_3 Anion.

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In this study, we successfully reproduced the photoelectron spectrum of P_2N_3 anion and its five electronic states by employing ab initio electronic structure calculations and quantum dynamics methods. These methods included time-dependent (TD) and time-independent (TI) quantum dynamical investigations. The Vibronic Hamiltonian, accounting for the coupling between electronic and vibrational motions, was constructed to facilitate these studies.

Our detailed analysis revealed that the photoelectron bands exhibited significant nonadiabatic effects. These effects arise from numerous conical intersections (CIs) and crossings among the electronic states, which are crucial in the system's dynamics. Conical intersections, where potential energy surfaces intersect, lead to rapid changes in electronic states, significantly affecting the observed spectra.

By accurately modelling these interactions, our theoretical bands, corresponding to the five electronic states of P_2N_3, closely replicated the experimental spectral bands. The results are illustrated in **Fig. 1**, where the X, A, B, and C states form combined peaks, while the D state forms a distinct individual peak. This close match indicates that our methods reliably predict the system's complex behaviour. The agreement between experimental results and our computational predictions, achieved using both TD and TI approaches, underscores the robustness of our approach in capturing the intricate details of the photoelectron spectrum. This study highlights the importance of including nonadiabatic effects and conical intersections in theoretical models to describe the electronic properties of complex molecular systems accurately.

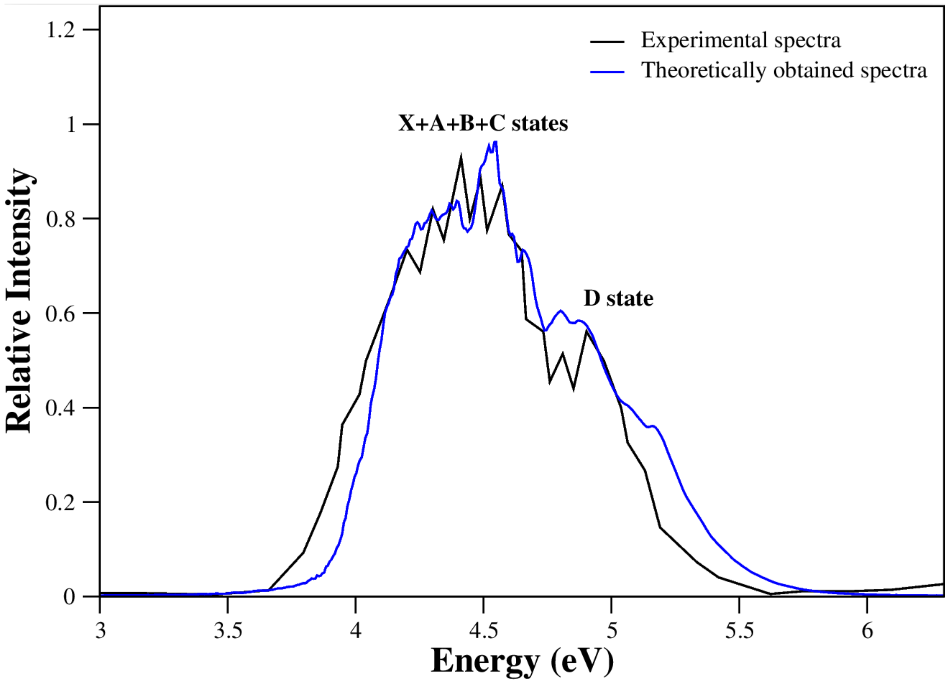

Fig.1 Comparison between experimental and theoretically obtained photoelectron spectra of P_2N_3 anion.

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G-122

Theoretical Study of the Structure and Vibrational Sum Frequency Generation Spectroscopy of Liquid-Vapour Interface of Aqueous Acetic Acid

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We investigated the liquid-vapour interface of aqueous acetic acid, a weak acid whose dissociation may be ignored. We have employed the electronic structure/molecular dynamics (ES/MD) approach [1, 2] coupled with vibrational sum frequency generation (VSFG) spectroscopy to examine the structure of hydrogen bond network of water at the liquid-vapor interface [3, 4]. The effect of concentration of acetic acid (AA) on the bulk and interfacial structural properties is also studied. Our findings show surface propensity of AA molecules and as the concentration of AA increases, the more AA molecules cover the interfacial region. The acetic acid molecules at the interface are found to be oriented such that the hydrophobic part (methyl chain) is oriented towards the vapour phase and the hydrophilic part is oriented towards the liquid phase. The total VSFG spectrum reveals that the intensity of the dangling peak of OH mode of water around 3750 cm−1 decreases, while the intensity of a peak around 3550 cm−1 due to hydrogen bonds between water and AA molecules, increases. Furthermore, this peak is redshifted as the AA concentration increases, which is due to the cancellation of the positive response of water OH modes by the negative response of the OH mode of AA. It is also noted that AA molecules make the interfacial water more structured by making hydrogen bonds with its dangling OH mode.

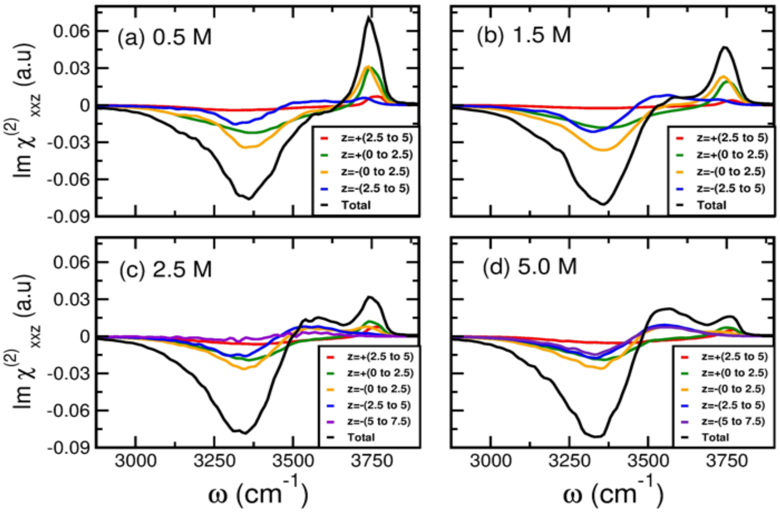

Figure1: The VSFG spectral contributions from different layers to the total VSFG spectrum for (a) 0.5M (b) 1.5M (c) 2.5M (d) 5.0M aqueous acetic acid.

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G-123

Study of $Mn_{n+1}B_{2n}$ (n = 1, 2, 3) MBenes towards Antiferromagnetic Properties

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Two-dimensional (2D) magnetic materials exhibit unique quantum mechanical phenomena and chemical properties due to intrinsic magnetism. Specially, 2D antiferromagnetic (AFM) materials have huge potential for future spintronic applications. Due of their vanishing magnetization, they do not produce stray field and also insensitive to external magnetic perturbation [1]. Here, we have explored the 2D manganese borides (known as MBenes) which are obtained from their bulk layered metal borides known as MAB phase (Here M=Mn, A=Al/Ga/In) after etching of A layer. The calculated lattice parameter and bond length of 2D $Mn_{n+1}B_{2n}$ is listed in Table 1 and the bond between Mn-B and B-B narrowly affected after etching of Al layer. Thermal, mechanical and dynamical stabilities of $Mn_{n+1}B_{2n}$ (n = 1, 2, 3) MBenes monolayer were estimated by formation energy, stiffness constant and phonon dispersion curves, respectively using spin-polarised density functional theory (DFT+U) (U =5 eV for present work) calculations within Quantum Espresso Simulation package [2]. Mn_2B_2, Mn_3B_4 and Mn_4B_6 MBenes monolayer are found to be antiferromagnetic metal with atomic magnetic moments of Mn site as 3.13, 2.86 (2.48) and 2.85 (2.63) μ_B/Mn-atom, respectively. Furthermore, the valence electrons are generally localised near the B-B chain in the unit cell of all MBenes monolayer, which show good structural stability of MBenes monolayer. Due to good structural stability and large atomic magnetic moment, 2D $Mn_{n+1}B_{2n}$ MBenes monolayer are promising candidate for next-generation spintronic device applications.

Table 1: Lattice parameter and Bond length of MAB phase and MBenes.

Compound	**Lattice Constant (Å)**			**Bond Length (Å)**							
	a	**b**	**c**	**Mn_1-B_1**	**Mn_1-B_2**	**Mn_2-B_1**	**Mn_2-B_2**	**Mn_2-B_3**	**B_1-B_2**	**B_2-B_3**	**Mn_1-Al**
Mn_2AlB_2	2.89	11.07	2.83	2.13	2.17	-	-	-	1.75	-	2.58
Mn_2B_2	2.91	2.86	-	2.11	2.17	-	-	-	1.79	-	-
Mn_3AlB_4	2.94	2.84	8.15	2.15	2.15	2.29	2.22	-	1.74	1.74	2.59
Mn_3B_4	2.87	2.84	-	2.05	2.01	2.40	2.19	-	1.79	1.72	-
Mn_4AlB_6	2.95	21.47	2.87	2.16	2.14	2.29	2.24	2.26	1.74	1.72	2.61
Mn_4B_6	2.87	2.90	-	2.07	2.01	2.41	2.22	2.26	1.79	1.70	-

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G-124

DFT Study On The Spin States Of Polyaniline–3d Transition-Metal (Sc–Zn) Composites And Their Sensing Application To Detect Chemical Warfare Agents

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Chemical warfare agents, or CWAs, have long posed a threat due to their terrible consequences for both the environment and human health. Inhalation of these dispersed aerosols is extremely poisonous. Due to their severe toxicity, there is an urgent need for the minute detection of these compounds.[1] Since, the polymer-metal composites possess the mechanical flexibility, electrical and optical properties of conducting polymers, along with the high electrical conductivity and magnetic properties of metals, they have attracted the attention of scientists for their application in optoelectronic devices and ultrasensitive chemical and biological sensors.[2] Further, the high surface area-to-volume ratio of the metal nanoparticles makes them particularly attractive for catalysis.[3] Thus to design such polymer metal composites, we combined polyaniline (PAni) with 3d transition metal (TM) atoms and investigated various spin states by performing density functional calculations. PAni polymer is unique among other conducting polymers because of its ease of preparation, environmental stability, low cost, controlled electrical conductivity, and intriguing redox characteristics.[4] These designed composites were analyzed for their stability in different spin states and their calculated electronic properties, including binding energies, frontier molecular orbitals, and dipole moments. The stable composite is further analyzed for its efficiency in sensing hazardous CWAs, such as hydrogen cyanide (HCN), cyanogen chloride (NCCl), cyanogen bromide (NCBr), cyanogen (NCCN), and arsine (AsH_3). The reduced band gap and significant red/blue shift in the UV–vis spectra obtained through TDDFT calculations underline the selectivity and efficiency of the Mn@PAni composite toward different analytes. The following graphical abstract (Fig. 1) depicts the observations of the theoretical calculations done on PAni-metal composites.[5]

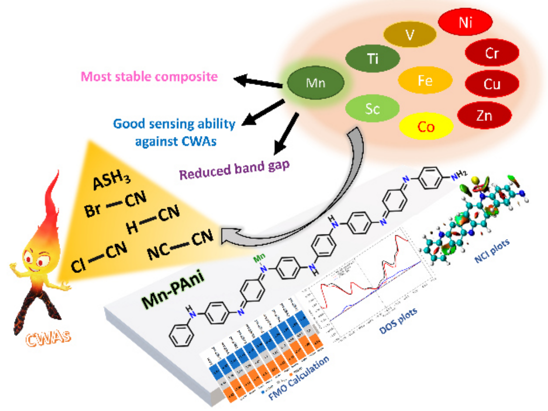

Figure 1. DFT calculations on PAni-metal composites depicting Mn-PAni as the best sensor for CWAs.

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G-125

Aggregation Behavior in Porphyrin Tautomer Variants: A Theoretical Study

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Recent advancements in density functional theory (DFT) and semi-empirical Hamiltonians have greatly enhanced the accuracy of supramolecular computational predictions, enabling precise molecular tuning for new materials. This study focuses on porphyrin, particularly *N*-confused tetraphenylporphyrin (NCTPP) and its tautomers, known for their unique aggregation patterns and promising photophysical and optoelectronic properties.[1] Understanding the intermolecular interactions among these molecules is crucial for designing materials with desired characteristics in supramolecular chemistry, material science, and related fields.[2] These interactions result in the formation of two distinct forms, the J form and H form, characterized by their differing geometrical arrangements. The predictive abilities of computational techniques for supramolecular systems have been reinforced by the latest developments in semi-empirical. Among these methods, Extended Tight Binding (xTB) stands out for its ability to strike a balance between accuracy and computational cost when determining dimer geometries and interaction energies. The interaction energy calculations are calculated using the Symmetry-adapted perturbation theory (SAPT). Moreover, electronic properties of these aggregates are assessed using time-dependent density functional theory (TD-DFT). Comparison with monomers and experimental data reveals that TD-DFT yields results that align well with experimental observations, particularly in terms of energy levels and non-covalent interaction energies. This comprehensive approach provides valuable insights for material design based on these properties.

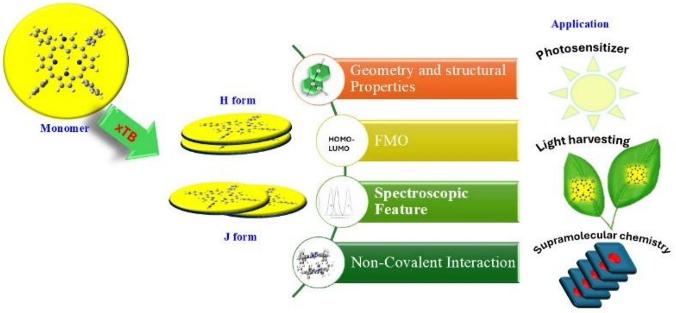

Figure 1: A schematic overview of the dimer analysis method and its applications

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G-126

Selectivity and Switchability of Hot Spot Activation in Nanolens-like Nanosphere Heterotrimers

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Near-field coupling between metal nanoparticles creates regions of strongly confined electric fields at the junctions of the particles, known as hot spots [1]. Nanoparticle assemblies with multiple hot spots offer opportunities for optical control. Linear trimers of self-similar nanoparticles with a hierarchical arrangement of monomers in terms of particle size along the chain, often explored as nanolens configurations, focus electromagnetic energy in the vicinity of the smallest particle [2-5]. In contrast with the traditional nanolens configurations, the current study embarks on an exploration of the optical control of hot spots using nanolens-like trimers of nanospheres with compositional asymmetry and with a constant gap size using finite-difference time-domain (FDTD) method. FDTD simulations were performed using the FDTD: 3D Electromagnetic Simulator software, a product of Lumerical Inc., Vancouver, Canada [6]. We analyzed the optical control features of a plethora of dimeric and trimeric configurations by examining their electric field intensity distribution profiles at their extinction maxima. Of the six trimeric systems considered, two of them were found promising for achieving selective excitation of hot spots, while two others were found useful for accomplishing hot spot switching. For the systems demonstrating optical control features, a wavelength dependence study was conducted by exciting them at two commonly employed laser wavelengths, namely 420 nm and 633 nm. Our simulations exemplify that a balanced choice of composition and size in the proposed nanolens-like configurations entails them with considerable optical control of hot spots, [7] a prediction that is worth investigating in surface-enhanced spectroscopy experiments.

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G-127

Structure and Properties of Unsubstituted/Di-methyl Substituted-Pyrazinyl Diselenide Anions

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In recent years diselenides have received significant attention for their possible biological and pharmacological use, due to their strong antioxidant properties. One electron reduction of neutral diselenides leads to weakening of chalcogen–chalcogen bond. The additional electron in such systems is accommodated in the lowest unoccupied molecular orbital which is often an antibonding sigma orbital [1]. In present work, electron acceptor properties of bis(2-pyrazinyl)diselenide [(2-pyzSe)$_2$] and bis(2,5-dimethyl-3-pyrazinyl)diselenide [(2,5-Me2-3-pyzSe)$_2$] have been investigated for their potential utilization as anti-oxidants [2].

The ground state properties of these compounds were estimated using electronic structure calculations as adopted in GAMESS program package [3]. For optimization, we have used hybrid functional (B3LYP) along with an all electron basis set as described in def2-TZVP. Both gas-phase model and polarizable continuum model were used for optimization of the geometric and electronic structures.

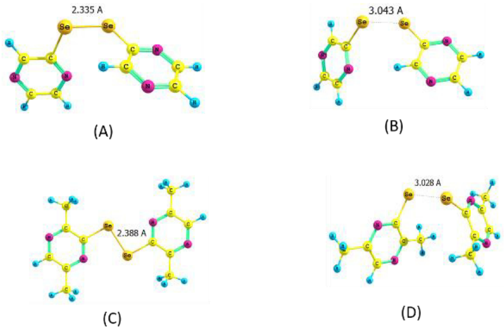

Figure 2 Most stable equilibrium structure of (a) pyrazinyl diselenide (b) pyrazinyl diselenide anion (c) di-methyl substituted-pyrazinyl diselenide and (d) di-methyl substituted-pyrazinyl diselenide anion, in water medium

Figure 1 depicts most stable equilibrium structures for neutral and radical anions of diselenide derivatives. For radical anions, elongation of Se-Se bond has been observed. The electron affinity of [(2-pyzSe)$_2$ and [(2,5-Me2-3-pyzSe)$_2$ has been estimated to be -3.38 eV and -3.33 eV respectively, in water medium. These values suggest that electron capture is a favourable process for these diselenide derivatives.

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G-128

Exploring the conformational space of sulfonyl anion based ionic liquid as a potential corrosion inhibitor on platinum based mono and bimetallic surfaces

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Managing the effects on metallic surfaces during and after chemical reactions, particularly in heat transfer processes or desalination, is a significant concern. The use of corrosive acids for surface cleaning leads to substantial corrosive damage. To address this issue, it is crucial to explore new corrosion inhibitors that can mitigate damage while maintaining low toxicity [1].

Ionic liquids, recognized as environmentally friendly solvents, also exhibit anti-corrosive properties. Investigation into the chemisorption of ionic liquids with varying activities demonstrates their effectiveness as corrosion inhibitors on metal surfaces [2].

This study focuses on exploring the potential of N-methyl-N-butyl-pyrrolidinium bis(trifluoromethylsulfonyl)imide as a corrosion inhibitor on platinum-based mono and bimetallic surfaces. Through temporal replica exchange molecular dynamics simulations, various configurations of the ionic liquid ion-pair were generated on the surface. Clustering analysis identified unique representatives of these structures, whose adsorption energies were calculated using density functional theory. The structures' uniqueness was further validated using the Smooth Overlap of Atomic Positions (SOAP) descriptor method, as shown in figure 1. Results indicate strong chemisorption of the bis(trifluoromethylsulfonyl)imide anion with the surfaces, while the cation undergoes multiple conformational changes, resulting in stable conformers of the ion-pair on the surfaces. The stability of this complex system suggests its potential as a corrosion inhibitor, as supported by the adsorption energies.

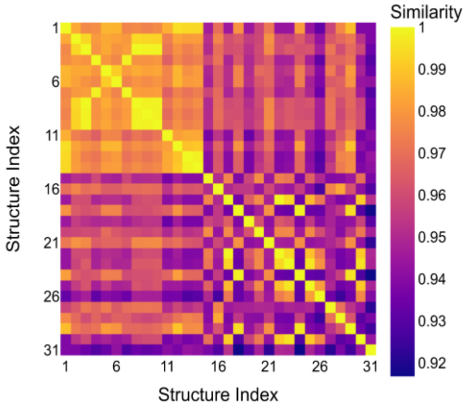

Figure 1: Similarity heatmap of the conformational space of ionic liquid adsorbed on metal surface

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G-129

Coupling of the Structure and Magnetism to Spin Splitting in Hybrid Organic-Inorganic Perovskites

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The ability to couple structural, electric and magnetic degrees of freedom to materials properties is of tremendous scientific and technological importance. For example, coupling between structural and electron spin degrees of freedom is promising for applications in spintronics. One of the ways to access spin degrees of freedom is through spin–orbit interaction, which breaks the Hamiltonian symmetry and splits spin-degenerate bands. Spin–orbit interactions in solids give origin to the so-called Rashba and Dresselhaus effects, which originate from structural inversion asymmetry and bulk inversion asymmetry, respectively [1]. These effects give origin to spin splitting in the electronic bands and, consequently, the opportunity to access a particular spin channel and also lead to the emergence of spin texturing in either real or reciprocal space. Certain types of spin textures are known to enhance spin states' lifetimes and, therefore, are critical for applications in spintronics. Spin splitting leads to spin-momentum locking, which manifests in the existence of spin polarizations in momentum space or spin textures. Such spin-momentum locking is highly desirable for spin-charge interconversion and could find applications in spintronics and quantum computing. In ferroelectrics, spin textures could couple to the electric polarization, which is known as ferroelectricity Rashba effects cofunctionality. Such coexistence allows for the control of spin-momentum locking by the external electric field [2-3].

Structural degrees of freedom are typically associated with ionic positions and lattice vectors and can be manipulated through temperature and external fields. Ferroics usually offer great opportunities for structural manipulations, as they have a tendency to undergo phase transitions and often couple to electric fields. Magnetic degrees of freedom are usually associated with localized spins and may be either disordered or ordered. Examples are paramagnetism and (anti) ferromagnetism, respectively. While ferromagnetism results in spin-dependent electronic band structures, more subtle effect of spin splitting has been predicted from group theoretical analysis in antiferromagnetic (AFM) materials. Remarkably, some AFM materials can exhibit spin splitting even in the absence of spin–orbit interactions. Recently, a novel class of magnetic materials known as altermagnets has emerged. These materials are collinear antiferromagnets, where spin sublattices are connected by proper or improper spatial rotation operations and exhibit spin splitting in their electronic bands in the momentum space, in the absence of spin–orbit coupling (SOC). It appears that materials in the ferroic, or more precisely multiferroic, family may have significant potential for coupling structure and magnetic ordering to spin splitting. [2-3]

With the help of first-principles simulations, we find spin splitting in both conduction and valence bands of $[NH_2NH_3]Co(HCOO)_3$ induced by spin−orbit interactions, which can reach up to 14 meV. The direction of the associated antiferromagnetic order parameter is strongly coupled with spin splitting in the centrosymmetric phase, allowing for the creation and annihilation of spin splitting through the application of a magnetic field. Furthermore, the structural phase transition to the experimentally observed polar $Pna2_1$ phase completely changes the aforementioned spin splitting and its coupling to magnetic degrees of freedom. This reveals that in $[NH_2NH_3]Co(HCOO)_3$, the structure and magnetism are strongly coupled to spin splitting and can be manipulated through electric and magnetic fields [1]. We believe that our findings offer an important step toward a fundamental understanding and practical applications of materials with coupled properties.

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G-130

Effect of *meso*-Pentafluorophenyl Group on Two-Photon Absorption in Heterocorroles andHeterocorrins

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Our work critically investigated the general notion that perpendicularly oriented *meso*-aryl substitutions in heterocorroles and heterocorrins do not affect their photophysical properties. To this end, we employed the state- of-the-art RICC2 method to study charge transfer and two-photon absorption (TPA) in 52 heterocorroles, heterocorrins, and their *meso*-pentafluorophenyl (PFPh) substituted analogues. Fig. 1 illustrates the said PFPh substitution scheme for Corrole and Corrin bases. The ground state geometries of all the considered systems are optimized using DFT [B3LYP hybrid functional and 6-311+G(d,p) basis set] level of theory, whereas the excited state properties (Transition dipole moments, OPA, TPA) are calculated at RICC2 [cc-pVDZ basis set] level of theory. Our observations revealed that PFPh substitution caused significant changes in the transition dipole moments corresponding to the first three singlet states, thereby substantially increasing the system's TPA strengths. To pinpoint which transition dipole strengths are involved and the effect of their orientation, we employed a four-state model within generalized few state model, which revealed that the TPA mechanism in some corrins differs from that in structurally similar corroles. This study helps in improving our understanding about the effect of *meso*-substitutions on charge-transfer and TPA mechanism of corrole and corrin systems. This might further help in designing corrole and corrin-based system for nonlinear optical applications.

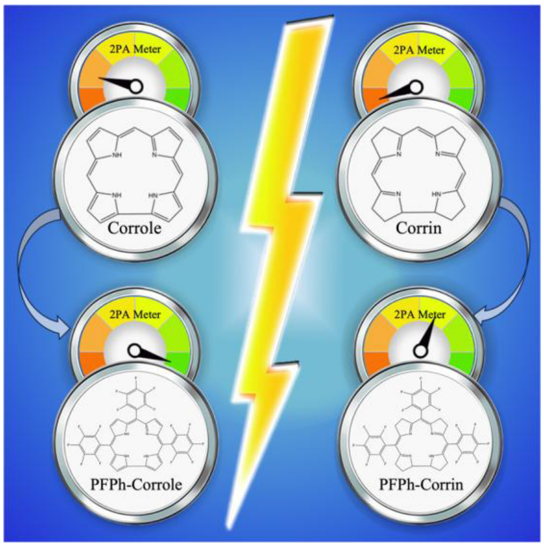

Figure 1 : Illustration of PFPh substitution scheme for Corrole and Corrin bases along with a schematic representation of the effect on two-photon absorption strengths as a result of *meso*-PFPh substitution.

G-131

Exploring Noncovalent Interactions Between Aromatic Heterocycles And Formic Acid: A Quantum Chemical Approach

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Understanding the significance of five-membered heterocycles and their weak bonding interactions is crucial for advancing our knowledge in biological and chemical systems, as these heterocycles are integral components of many biologically relevant molecules [1]. In this investigation, we utilized different quantum chemical approaches to elucidate the noncovalent interaction between aromatic heterocycles (XC_4H_4, where X=O, S, Se) and formic acid (FA). Study reveals that furan prefers to bind with formic acid through its nonbonding electrons on the O atom, while thiophene and selenophene do so through their π electron cloud in the molecular system. The interaction energy calculated using both the symmetry-adapted perturbation theory and supermolecular approach follows the trend: $FA{\cdots}OC_4H_4 > FA{\cdots}SeC_4H_4 > FA{\cdots}SC_4H_4$. This computed interaction energy is highly influenced by electron correlation and basis set size. The dimers primarily stabilized by electrostatic and dispersion forces are engaged in charge transfer from the nonbonding and π-orbital of the aromatic heterocycle moieties to the antibonding orbital of the O-H bond in FA. Additionally, the topological analysis of electron density confirms the presence of closed-shell interactions, notably moderate-strength hydrogen bonding in the dimeric complexes. These findings are consistent with the previously reported experimental work [2].

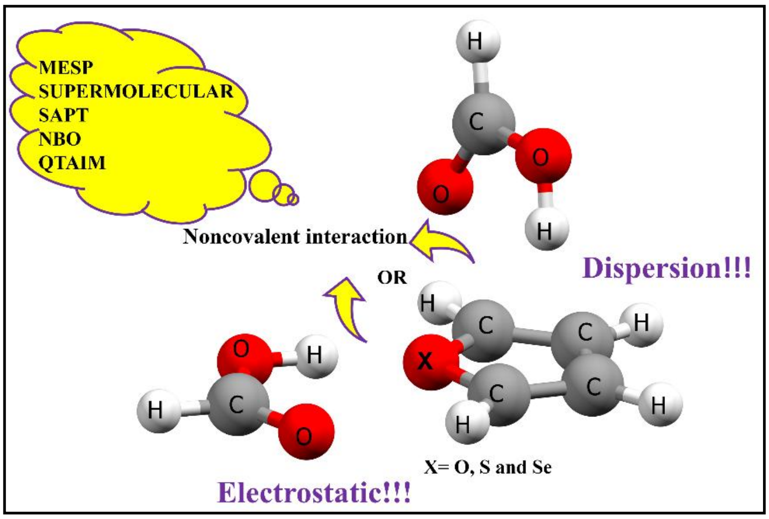

Figure 1: Noncovalent interaction of aromatic heterocycles: furan, thiophene and selenophene with formic acid

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G-132

Cooperativity Effects in Lithium-Hydride seeded Ammonia clusters

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The attractive forces between molecules are just strong enough to cause clustering, and resist on further compression to form condensed phases due to the repulsive forces; keeping the cluster fragments from reacting and preserving the chemical identity of the individual fragments composing the cluster. The role of noncovalent interactions in the cluster structure is thus very important. Recently, a new perspective governing the nature and strength of multiple noncovalent interactions have emerged, wherein these interactions mutually reinforce into each another as a phenomenon of cooperativity [1]. In the present study, we try to understand this phenomenon of cooperativity, in LiH seeded ammonia clusters and present a systematic study with an aim to understand the coexistence of these noncovalent interactions. ORCA [2] program package (version-5.0.4) has been employed for all quantum chemical calculations carried out in this work. Optimized molecular structures are calculated using RI-MP2 theory with 6-311++g(2df,2pd) basis sets, and the QTAIM analysis has been done using multiwfn. NBO program [3] is employed to obtain the 2nd order perturbation interaction energy $E^{(2)}$ along with the estimates s and p contribution to the natural hybrid orbitals (NHOs).

Tab. 1 Natural Bond Analysis of the LiH seeded NH_3 clusters $LiH(NH_3)_n$ with n=1 to 3

n	**Donor (i)**	**Acceptor (j)**	**E (2) (kcal/mole)**	**Distance, r (Å)**		**NHOs**	
1	LP (1) N1	LP*(1) Li5	25.91	N1---Li5	2.047	$SP^{3.46}$	$SP^{2.32}$
2	LP (1) N1	LP*(1) Li9	25.39	N1---Li9	2.046	$SP^{3.77}$	$SP^{0.95}$
	LP (1) N5	LP*(1) Li9	25.4	N5---Li9	2.046	$SP^{3.77}$	$SP^{0.95}$
	σ (Li 9 - H10)	σ*(N5 - H8)	0.34	H8---H10	2.556	$SP^{1.06}$	$SP^{2.76}$
	σ (Li9 - H10)	σ*(N1 - H4)	0.34	H10---H4	2.556	$SP^{1.06}$	$SP^{2.77}$
3	LP (1) N1	LP*(1) Li13	22.8	N1---Li13	2.073	$SP^{4.02}$	$SP^{0.57}$
	LP (1) N5	LP*(2) Li13	23.72	N5---Li13	2.073	$SP^{4.02}$	$SP^{1.00}$
	LP (1) N9	LP*(1) Li13	22.82	N9---Li13	2.073	$SP^{4.02}$	$SP^{0.57}$
	σ (Li13 – H)	σ*(N9 - H12)	3.86	H---H	2.107	$SP^{1.78}$	$SP^{2.83}$
	σ (Li13 – H)	σ*(N5 - H8)	3.87	H---H	2.107	$SP^{1.78}$	$SP^{2.59}$
	σ (Li13 – H)	σ* (N1 - H3)	3.87	H---H	2.107	$SP^{1.78}$	$SP^{2.58}$

The results of NBO analysis (Tab. 1) carried out on $LiH(NH_3)_n$ (n=1-3) elucidates the extent of hyper-conjugation and or intramolecular delocalization. Estimates of $E^{(2)}$ suggests that the (Li---N) lithium bonds largely contribute to the stability of $LiH(NH_3)_n$ clusters followed by the (N-H---H-Li) dihydrogen bonding. Moreover, these results indicate that average interatomic distances between N-H, Li-H, and Li---N increase, and a new non-conventional hydrogen bond [3] emerges as more ammonia molecules gets added. We compare our results with the recent work on pure NH_3 clusters [4] and find that LiH in NH_3 results in copious non-covalent interactions causing redistribution in electron density, which upon reinforcement develops possibility of cooperativity among these interactions. The QTAIM analysis, further supports this observation revealing that the electron density at the bond critical points for interatomic distances r(Li-H) and (Li---N) decreases as the distance between these atoms increase.

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G-133

Effect of Iodine, and Polar Group Substitution at *α*, *β*, and *meso*-Positions on the Quality of BODIPY-based TP-PDT Photosensitizers

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BODIPY-based photosensitizers are well-known for their two-photon activity. There are three different locations, namely *α*, *β*, and *meso* (as shown in Figure 1) where the BODIPY core can be substituted with various groups. As found in the literature, the *meso* position is one of the most favored positions for substitutions. This is probably because of its labile nature and hence ease of synthesis. There is no systematic study revealing the effect of positions of the substitutions on the TP activity of BODIPY systems. Furthermore, we have found that there is no report on the effect of heavy atoms such as iodine on the said property. To fill these gaps, in this work, we present a systematic study of the effect of heavy atoms, and that of the position of polar group substitutions in the BODIPY core on TP activity. For this purpose, we considered two BODIPY cores (one with Iodine substitution at the β position BDPI2 and the one without this substitution BDP1). These BODIPY cores are substituted at the remaining positions (one by one) by six different polar groups resulting in a total of 36 systems (18 for each core). The one- and two-photon absorption in all these systems are studied at the RI-CC2 level of theory. The four systems (two from BDPI2 and two from BDP1) having the largest TP activity are chosen to get further insight into the two processes using a four-state model. Furthermore, these four systems are used for studying the docking and interaction of BODIPY with human serum albumin protein. Autodock Vina and Gromacs are used respectively for these studies. Our results suggest that the introduction of iodine and incorporation of polar groups at the α-position enhances the TP activity in both BDPI2 and BDP1 systems.

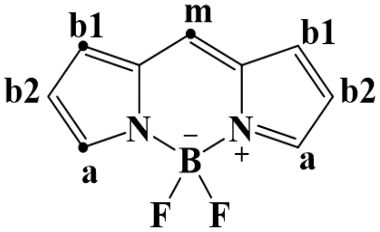

Figure 1. The schematic illustration of α, β, and *meso*-positions of the BODIPY core (α, β, and *meso*-positions abbreviated as a, b, and m respectively).

G-135

Tuning The Anti-aromatic Character for Stability: A Quantum Mechanical Approach

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Pentalene does not exist in nature as such due to its anti-aromatic character which render it highly unstable. But it was observed that when two aromatic rings, for example benzene, were introduced to the pentalene core, it stabilized the pentalene core. The stabilization occurred despite the new molecule being anti-aromatic. In this work, we have aimed to provide the theoretical understanding of the stability of DBP (Dibenzo-pentalene) by calculating HOMO-LUMO Energy Gap (ΔE_{HL}), Harmonic Oscillator Model of Aromaticity (HOMA), Bird Aromaticity Index, Aromatic Fluctuation (FLU-π) index and ^{1}H NMR properties [Figure 1] for these structures with the help of Density Functional Theory (DFT).

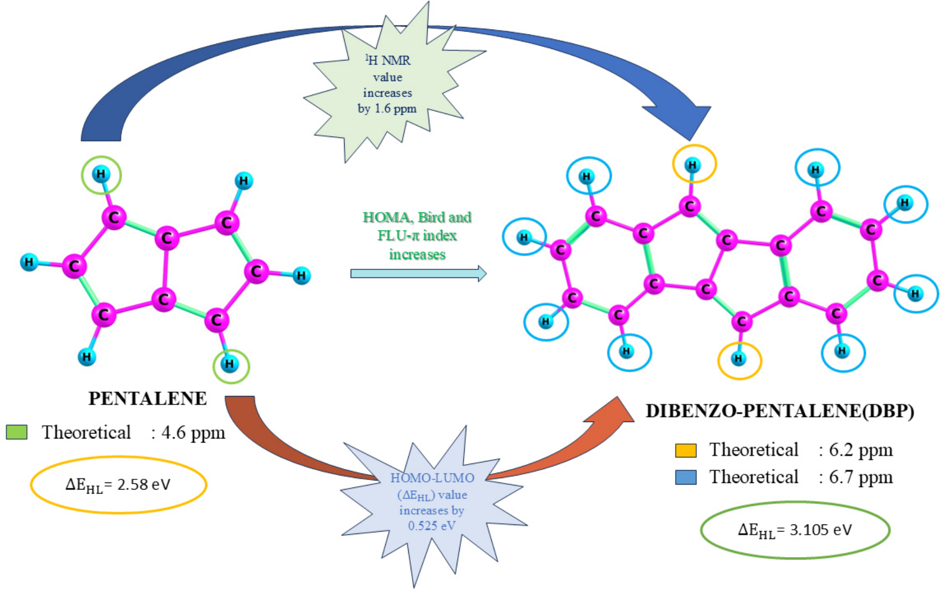

Figure 1. Reduction of anti-aromatic character as shown by the increase in the value of ^{1}H NMR, HOMA, Bird and FLU-π index by going from pentalene to DBP

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G-136

Stability of Cubic Nanoclusters Under Different Solvent Environments

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Nanoclusters (NCs) are molecular associations of a few to several hundred atoms in the 1-3 nm diameter range. These substances possess distinctive physical and chemical characteristics that are employed in a wide range of applications such as catalysis, magnetic storage, sensors, and biological markers. Due to the fact that size and shape are inherent characteristics, they have a significant impact on the capabilities of the structures[1]. Due to their unique properties like high surface area to volume ratio, nanocubes with sharp edges have garnered attention enabling them to be used in bioimaging and drug delivery[2]. While cubic morphologies are predicted to have enhanced applications, their weaker stability makes them more challenging to synthesize than spherical geometries.

Stability of Gold, Silver and copper cubic nanoclusters with different sizes from 14 to 1099 atoms in the presence and absence of 4 M [N1114][C1SO3] ionic liquid (IL) was assessed using molecular dynamics study. Both in the presence and absence of IL, larger NCs with more than 256 atoms exhibited stability compared to their smaller counter parts due to large metal-metal interactions. These less stable NCs could be stabilized in the presence of IL as they weaken the metal-water interaction thereby retaining the structure of smaller NCs[3].

While examining the small metal NCs with 63 and 108 atoms, it was found that the copper NCs showed weaker interactions with water which helped them to retain their structure compared to gold and silver NCs whose interaction with water was very high. Copper NCs were stable even in the absence of IL. Also any NCs with size less than 63 atoms were not stable even in the presence of IL which makes their sysnthesis challenging.

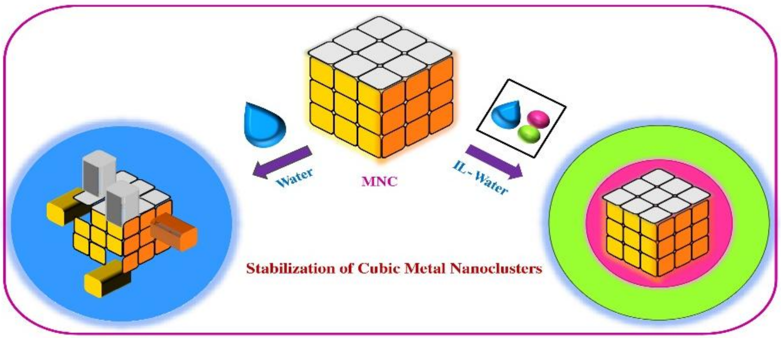

Figure 1. Metal nanoclusters exhibited greater stability in the presence of 4 M [N1114][C1SO3] ionic liquid solution

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G-137

Construction of Beyond-Born-Oppenheimer Based Diabatic Potential Energy Surface: Naphthalene Radical Cation

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First-Principle-based Beyond Born Oppenheimer (BBO) theory [1-3,5] is applied to a realistic molecular system, specifically the naphthalene radical cation (Np^+) to generate diabatic potential energy matrices, to compute the photoelectron spectra of the neutral analogue. Intense non-adiabatic coupling among the lowest six electronic states of $C_{10}H_8{}^+$ across twelve normal modes in the Franck-Condon region significantly influences the spectral features of the molecule.[4] We have employed Complete Active Space Self-Consistent Field (CASSCF) and Coupled-perturbed Multi-Configurational Self-Consistent-Field (CP-MCSCF) level of electronic structure theory to calculate the *ab-initio* adiabatic potential energy surfaces (PESs) of the six electronic states and the non-adiabatic coupling terms among those states, respectively using an 11 electrons 6 orbital (11e,6o) Complete Active Space (CAS) . The numerical instability originating from the singularity of NACTs is removed by performing the Adiabatic to Diabatic Transformation (ADT), thereby generating the ADT quantities (ADT angles and matrices) and the diabatic PESs for the molecular system. Wave packet dynamics using the Time-Dependent-Discrete-Variable-Representation (TDDVR) formalism shall be carried out on the above mentioned diabatic surfaces to calculate the theoretical photoelectron spectrum of the molecule.

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G-138

Ground and Excited State Molecular Properties Calculation by Employing the Four Component Relativistic Unitary Coupled Cluster Theory

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The accurate calculation of molecular properties in both ground and excited states is essential for understanding the behavior of molecules, especially in systems where the relativistic effects are significant. Due to the variational and non-hermiticity nature of the wave function of traditional coupled cluster theory[1], one needs to solve an extra set of amplitude equations for the ground state and additionally, one extra set of eigenvectors needs to be solved for the excited state molecular property calculations, that makes the calculation computationally very expensive. So, the unitary coupled cluster makes an advantage over this computationally expensive due to its hermitian nature of the wave function and because of hermiticity one needs to solve only one set of amplitudes and additional one set of eigenvectors to calculate the ground and excited state properties respectively. We have recently implemented a four-component relativistic unitary coupled cluster (UCC)[2] method for atoms and molecules. Where we have shown the spectra of Mg^{2+} ion in both relativistic and non-relativistic frameworks (see the figure below). We have presented a comparison of the excitation energy and transition dipole moment of Xe atom and compared it with the available experimental value. We have calculated the ground state molecular frame dipole moments of alkaline earth metal monofluorides and also calculated the hyperfine splitting and electric field gradient (EFG) value of some molecules and compared them with the Z-vector method of CCSD[3] method.

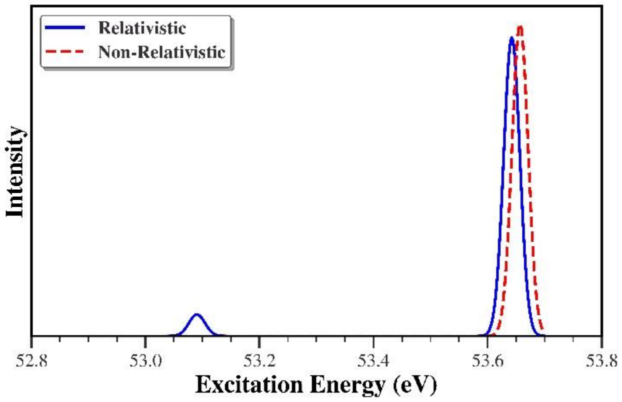

Figure 3: Absorption spectra of Mg^{2+} ion obtained from EE-UCC3 and EE-qUCCSD in the four component relativistic and non-relativistic frameworks

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G-139

Potential Catalytic Activity of Silver-Rhodium based Bimetallic Nanoclusters

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Abstract: Bimetallic nanoclusters exhibit beneficial characteristics as compared to their pristine constituent metal cluster, as the hybrid materials provide opportunities for inter-metallic interaction that can improve their catalytic properties. Moreover, their catalytic activity can be optimized by controlling the structural factors, such as the doping element and its concentration. Thus, understanding how the reactivity of these nanoclusters changes with the composition is highly essential for designing new catalysts. While designing a bimetallic nano catalyst, one has to consider various factors like stability of the structure, optimal ratio of the two atoms and binding energies of the adsorbent on various positions of the cluster. Theoretical methods are best suited for such studies as they help to obtain detailed information on the optimized configurations and mechanism of the reaction, which are not directly accessible to experiment. In the present study, we theoretically investigate the activation of Ag8 nanocluster by Rh doping, and its effect towards CO oxidation. Density functional theory-based calculations have been carried out to investigate the electronic structure theory of pure Ag8 and Rh8 clusters as well as Ag_xRh_{8-x} bimetallic systems, where x=1 to 7 and to explore their reactivity towards CO molecules. The differences in the behaviour of these clusters are analysed based on the concentration of the dopant electronic properties and binding energy of the adsorbents. As shown in Figure 1, the results indicates that Rh doping can activate the otherwise inactive Ag nanoclusters by increasing the adsorption energy almost 8 times. The increased catalytic activity of Ag_7Rh system for CO oxidation is due to enhanced charge transfer within the bimetallic system. The enhanced catalytic activity could be satisfactorily explained using ensemble effect. As the number of dopant atoms increased, the adsorption energy values gradually decreased and reached a saturation level.

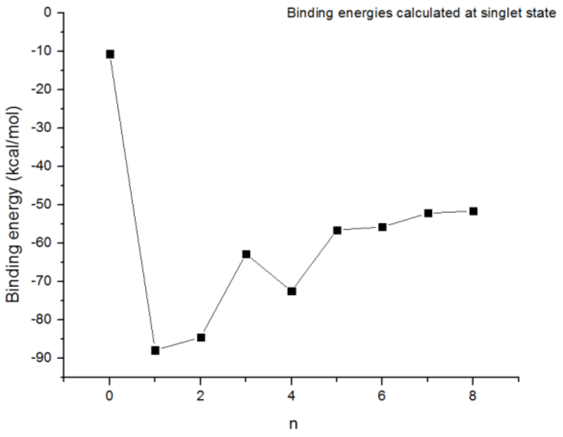

Fig: Variation in adsorption energy of Ag_xRh_{8-x} clusters at singlet states.

G-140

Optimisation of Copper oxide Nanotubes using Hybrid Density Functional Theory

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Copper oxide has been studied extensively experimentally as well as theoretically because of fundamental understanding and applied reasons. [1] It serves as a prototype system for broad family of strongly correlated oxides. CuO bulk assumes monoclinic structure with its band gap of 1.0-1.9 eV. The nanostructured CuO has shown wide range of applications in optoelectronics, spintronics, magnetic sensor etc. Among different nanostructure, CuO nanotubes have been explored for gas adsorption, biosensor for glucose detection etc. Though, CuO nanotubes has been experimentally explored, theoretical understanding of the nanostructure is less emphasised. In the present work, we have optimised the structure of CuO nanotubes of different diameter and electronic structure of the tubes are explored using hybrid density functional theory (HSE06).

Previously, we have optimised the structure of copper oxide clusters which shows planar ring like structure for trimer, tetramer, pentamer, hexamer and heptamer. [2] For optimisation of CuO nanotubes, these planar structures are arranged in layer form in staggered fashion. To stabilise the tube structure, at least 4 layers of each ring structures are required which become the unit cell of the CuO nanotubes. The optimised cell parameter for CuO nanotubes of n=3, 4, 5, 6, 7 are calculated to be 7.45, 7.75, 7.65, 7.70, 7.9 Å respectively. Subsequently, band gap for $(CuO)_3$, $(CuO)_4$, $(CuO)_5$ $(CuO)_6$, $(CuO)_7$ nanotubes are calculated to be 0.52, 0.68, 0.65, 0.47 and 0.46 eV respectively. As the band gap of the nanotubes are found to be small, they can be used for various application such as gas adsorption, catalysis etc.

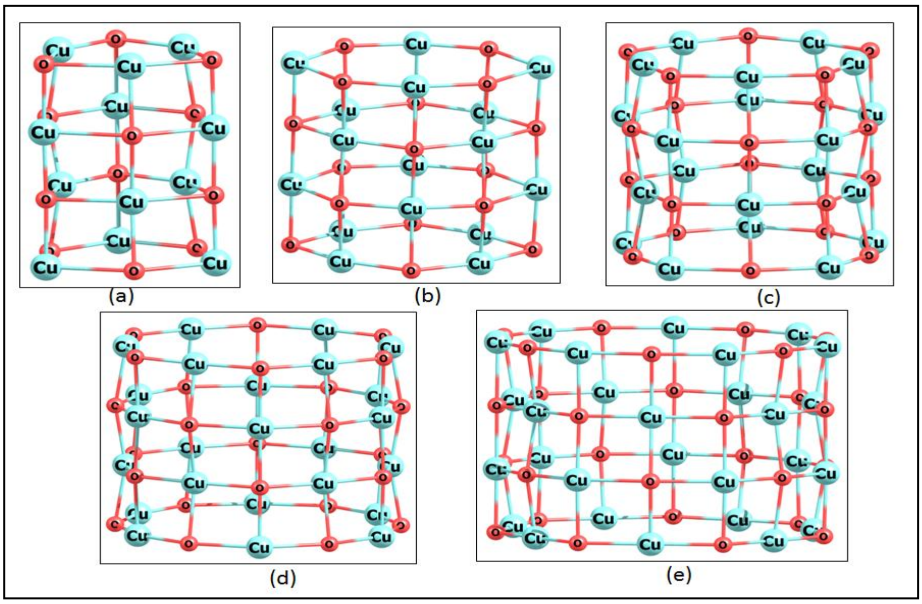

Figure 1: Optimised structure of CuO nanotubes comprised of (a) trimer (b) tetramer (c) pentamer (d) hexamer and (e) heptamer unit in vertically staggered orientation

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G-141

A Relativistic DFT Investigation of Uranyl Complexation with Bio-Compatible Pyrazine-2-Amidoxime

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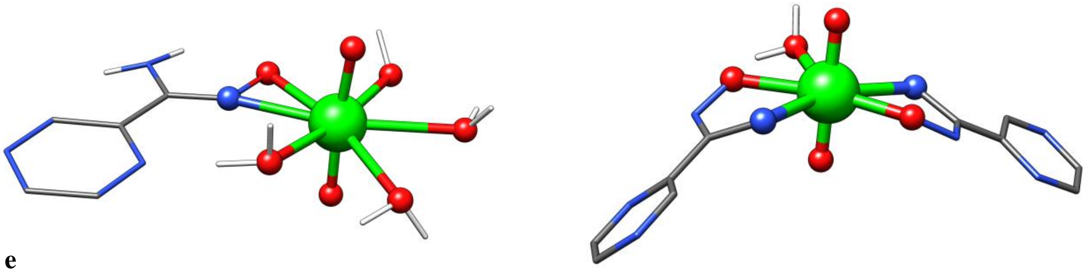
Uranium, while crucial for nuclear energy production, poses significant health risks upon accidental internalization in the human body, highlighting the need for effective decorporation agents.[1] Pyrazine-2-Amidoxime (PAOX), a bio-compatible chelator, has been explored for its potential to bind and remove the uranyl ion $[UO_2]^{2+}$. Using relativistic density functional theory (DFT), this study examined the structural and energetic properties of $[UO_2]^{2+}$ -PAOX complexes, showing that the 1:2 coordination mode is more stable than the 1:1 configuration, in agreement with experimental findings.[2] The stability of the 1:2 complex is enhanced by water molecules, which help satisfy the coordination requirements at the equatorial plane. Energy Decomposition Analysis (EDA) revealed that bonding in these complexes is primarily governed by electrostatic interactions, with notable contributions from orbital interactions. Furthermore, Quantum Theory of Atoms in Molecules (QTAIM) analysis demonstrated that the uranium-oxygen bond exhibits a predominantly covalent nature, whereas the uranium-nitrogen bond is more ionic, as reflected by lower electron density and a smaller Laplacian at the Bond Critical Point (BCP).[3] While computational results support the stability of these complexes, ongoing experimental studies are investigating the biological efficacy of PAOX as a decorporation agent.



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1. $[UO_2]^{2+}$-PAOX coordination modes in 1:1 and 1:2 manner

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H-121

Effect of Superhydrophilic Confinement on Solid-Liquid Coexistence of Water using Free Energy Analysis with mW Model

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Here, we investigate the effect of slit confinement on solid-liquid coexistence of water within strongly-hydrophilic slit pore size (H) varying from 8.5 Å to 70 Å, using Gibbs free energy analysis with monatomic water (mW) model [1]. Understanding the mechanism of water phase transformation is one of the greater interest among the researchers as water is the most abundant substance in all living organisms which plays an essential role in the survival of life, further calculations of thermodynamic free energies for phase transitioning systems are extremely important in studying a wide variety of chemical and biochemical phenomena including molecular solvation, macromolecular stability, protein folding, advancing drug discovery. We perform MD simulations (LAMMPS) in order to determine the solid-liquid coexistence or thermodynamic melting point by employing thermodynamic integration along with MHR (multiple-histogram reweighting) methods [2]. Gibbs free energy difference is computed using reversible and integrable pseudo-supercritical transformation path connecting the two phases. Each of the confined water systems is simulated for the three water-wall interaction strengths: $\varepsilon_{wf} = 1.0$, $\varepsilon_{wf} = 1.25$ and $\varepsilon_{wf} = 1.75910$. The estimated free energy difference is found to be different for the different confinement sizes as well as interaction strengths. The computed melting temperatures for H = 40 Å with $\varepsilon_{wf} = 1.0$, $\varepsilon_{wf} = 1.25$ and $\varepsilon_{wf} = 1.75910$ are 262.66 ± 1.3 K, 238.13 ± 1.3 K and 243.096 ± 1.3 K, respectively. While for H = 70 Å, the estimated melting temperatures with $\varepsilon_{wf} = 1.0$, $\varepsilon_{wf} = 1.25$ and $\varepsilon_{wf} = 1.75910$ are 252.48 ± 1.3 K, 246.24 ± 1.3 K and 248.68 ± 1.3 K, respectively [Fig. 1]. Oscillatory nature is observed in the melting temperature with the varying pore size, which is in well agreement with the previous literature. However, for all the pore sizes with all the three interaction strengths, the melting temperature is found to be lower compared to the recently reported melting point of bulk water. The study enthralls in attaining deeper insight into the mechanism of solid-liquid phase transition of water.

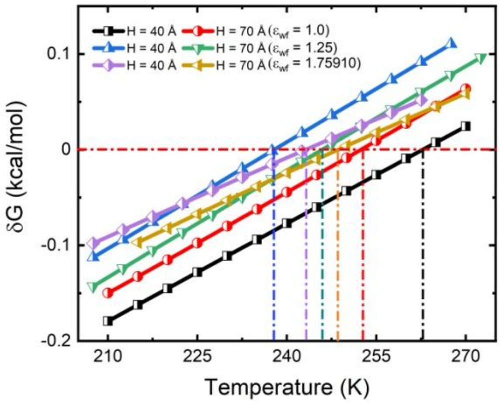

Figure 1. ΔG vs T for slit confinement pore sizes H = 40 Å and H = 70 Å with $\varepsilon_{wf} = 1.0$, $\varepsilon_{wf} = 1.25$ and $\varepsilon_{wf} = 1.75910$. The horizontal dash-dotted line implies where $\Delta G = 0$.

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H-122

The Formation and Implication of Hydrated Organic Volatile Compounds in the Atmosphere: A DFT Study

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A suspension of liquid or solid particles in a gas with particle dimensions between $10^{-9} - 10^{-4}$m is commonly known as an aerosol (lower limit: molecules and molecular clusters; upper limit: rapid sedimentation). Density functional theory has been used to compute the gas-phase geometries, binding energies, ZPE-corrected binding energies, BSSE-corrected binding energies, binding enthalpies, binding free energies of formaldehyde-(ammonia) -(water)$_{n,}$ acetic acid-(ammonia)-(water)$_n$, acetaldehyde-(ammonia)-(water)$_n$, and acetone-(ammonia)-(water)$_n$ cluster with n = 1-10, 15, 20, 25, and 30. The ZPE-corrected binding energies are computed at absolute zero kelvins (0 K) at the DFT/6-311++G(2d,2p) level of theory. Both binding energies and BSSE-corrected binding energies are calculated at 298.15 K and 1 atm(DFT: PW91PW91[1], M06-2X[2], ωB97x-D[3]). Enthalpies and free energies are calculated for a range of atmospheric relevant temperature (T) and pressure (P) (from T = 298.15 K, P = 1013.25 hPa to T = 216.65 K, P = 226.32 hPa). The outcome demonstrates that as temperature and pressure decrease, both enthalpies and free energies grow more negative. The optical properties of studied clusters have been studied at the CAM-B3LYP/aug-cc-pVDZ level of theory. The scattering intensities were calculated for naturally polarized light at static (∞ nm) and different wavelengths of 700, 600, 500, and 400 nm.

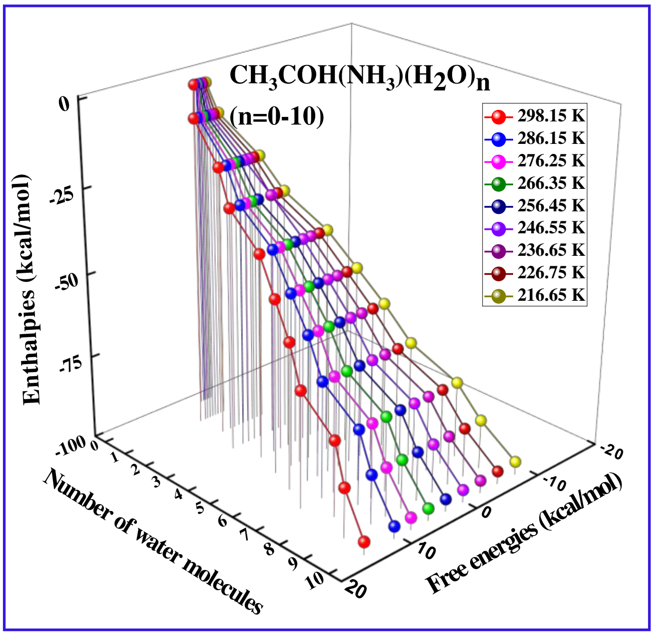

Figure 1. Binding Free energy and enthalpies of acetaldehyde-(ammonia)-(water)$_n$

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H-123

Investigations on $YbTaO_4$ Under Compression: First Principles simulations

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$YbTaO_4$, a compound of rare earth orthotantalate ($RTaO_4$) family, is recognized for its diverse range of applications due to its unique properties. Its high-temperature stability makes it suitable for use in high-temperature ceramics, where it can serve in aerospace, automotive, and other industrial applications that demand materials capable of withstanding extreme conditions [1]. The compound's electronic properties also position it well for use in solid-state devices, such as capacitors and sensors, where reliable performance is essential. $YbTaO_4$ like other compounds of $RTaO_4$ family, exhibits polymorphism depending on processing temperature, heating time and method of synthesis. Depending on processing parameters $YbTaO_4$ has been reported to synthesize in three types of monoclinic crystal structures with M fergusonite (*I*2/*a* SG: 15) and M' fergusonite (*P*2/*c* SG:13) and wolframite (*P*2/*c* SG:13) [2]. DFT based first principles calculations in GGA prescription are carried out on the M' phase of $YbTaO_4$ from ambient pressure to 50 GPa with an interval of 1 GPa using Quantum Espresso code [3]. Projector augmented wave (PAW) pseudopotentials for Yb, Ta and O atoms were taken from PSlibrary with 8×8×8 Monkhorst pack mesh grid and 100 Ry energy cut off while performing simulations. Unit cell parameters obtained from geometrically relaxed structure are in excellent agreement with published data. Figure 1 depicts the evolution of unit cell volume under compression. As shown in figure 2, under compression monoclinic angle starts deviating around 30 GPa and attains value close to 90 degrees around 43 GPa indicating possibility of isostructural phase transition in compound. Pressure evolution of simulated lattice parameters in ambient phase indicates anisotropic compression of unit cell with *b* and *c* axes being fourth times more compressible than *a* axis for the compounds due to structural arrangement of constitutional polyhedral units. Axial compressibility obtained by fitting the calculated lattice parameters to BM-EOS for $YbTaO_4$ are $K_a=0.8x10^{-3}GPa^{-1}$, $K_b=4.3x10^{-3}GPa^{-1}$ and $K_c=4.4x10^{-3}GPa^{-1}$. Similar behaviour has been reported in in other rare earth metal oxides $EuTaO_4$, $GdTaO_4$, $NdTaO_4$, $SmTaO_4$ under compression [4]. Bulk modulus obtained by fitting the pressure-volume data (figure 1) to 3rd order B-M equation yields a value of 101 GPa which is in good agreement with bulk modulus reported for the $RTaO_4$ family of compounds. Compressibility analysis of simulated volume of constitute polyhedral units YbO_8 and TaO_6 indicates that major contribution to the bulk modulus comes from RO_8 polyhedra which validates Hazen and finger proposed empirical model for predicting bulk modulus taking contribution from rare earth polyhedra unit as seen in RVO_4, RWO_4, $RMoO_4$ compound

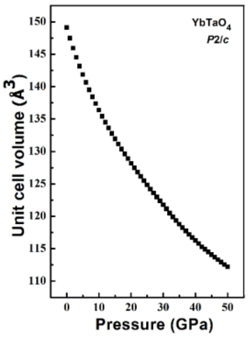

Figure 1. Pressure-volume data for $YbTaO_4$

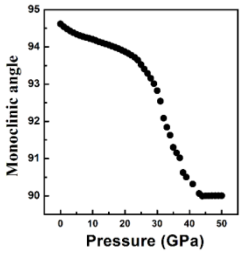

Figure 2. pressure evolution of β angle

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H-124

First-Principles Study of Titanite-Type $CaTiSiO_5$ under Pressure

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The titanite-type $CaTiSiO_5$ is widely recognized for its significance as a petrogenic indicator, a versatile host for rare earth elements (REE), and as a U-Pb geochronometer for dating geological events. Further, it is also a promising wasteform for the high level nuclear wastes. In ambient conditions, it exhibits a monoclinic structure (monoclinic-I, SG-$P2_1/c$). However, it shows phase transitions from the monoclinic-I (P21/c) phase to a monoclinic-II (C2/c) structure at higher temperature. In addition to these monoclinic forms, some titanite minerals are also well known for having a triclinic structure (SG-P$\bar{1}$). In this work, we have studied this phase under pressure ranging from 0-50 GPa. In this study, we have identified two new structural polymorphs at higher pressures using an evolutionary algorithm. Further analysis of their structural, elastic, and dynamical stability has revealed the pressure-dependent stability regions of these new polymorphs.
Evolutionary algorithms as implemented in USPEX package [1] was used for prediction of the crystal structures at high pressures. The structures at high pressure, initially, screened using USPEX package interfaces with classical force field. The structures which energies are within 2eV to the most stable structure are then optimized using density functional theory based calculations as implemented in VASP. PAW potentials [2] were used in all the calculations. The symmetry of the structures were analysed using VASPKIT software [3].
We have found $P2_1/c \rightarrow C2/c$ phase transition around 8 GPa by using DFT-PBE exchange-correlation functional however, no phase transition is observed in case of DFT-LDA functional. From the crystal structure prediction, we have predicted two new phases; one is triclinic (SG-$P\bar{1}$) at 10 GPa and another one is orthorhombic (SG-*Pnma*) at 20 GPa. The predicted triclinic structure resembles those structural prototypes found in other titanite minerals. In our calculations, both triclinic and orthorhombic structures are mechanically and dynamically stable. The orthorhombic structures which is quenchable at 0 GPa, possesses a novel topological rearrangement of SiO_6 and TiO_6 octahedra that has not been observed in any of the HP structural prototypes of silicate minerals.

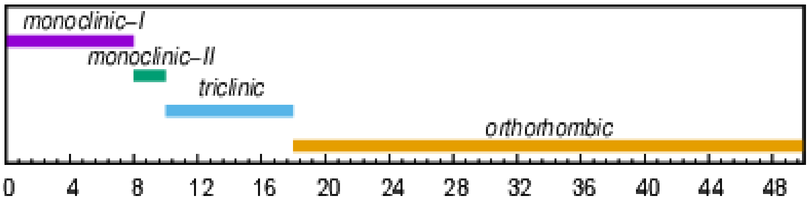

Figure 1: Stability region of different high pressure phases of titanite type $CaTiSiO_5$

High pressure crystal structures are predicted for $CaTiSiO_5$ composition. The new predicted triclinic and orthorhombic structures are mechanically and dynamically stable.

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H-126

Molecular Dynamics Insight of Ice Growth on Different Crystallographic Plane

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Ice growth on supercooled water has attracted attention because ice and water are very important for the environment and play very crucial roles in several natural processes. Hexagonal ice (I_h) is the most common and available form of ice among 18 known crystalline phases of ice. In this work we report the results of classical molecular dynamics study of ice growth on various planes of hexagonal ice. We have presented ice growth from super cooled water along three different planes of hexagonal ice namely basal and prismatic (primary and secondary) planes. Growth process for primary and secondary prism plane is quite similar where newly formed ice formation occurs in all possible direction as indicated by the rough nature of the growing surface with ultimate formation of only hexagonal ice with no stacking faults. On the other hand, growth phenomena from the basal surface are completely different. Here water molecules attach to the ice phase in a two-dimensional way rather than three-dimensional cluster formation as indicated by the nearly perfect planner growing surface). Growth process proceeds through the complete crystallization of the each 2D growing surface (layer-by-layer) along the growth direction. For the basal plane growth, formation of each layer occurs through nucleation phenomena probed by the halting nature at the initial of each layer formation. At the initial stage of the layer formation for each interface, we observe that both cubic and hexagonal ice is formed simultaneously up to the fractional coverage of ~ 0.2. After that there occurs a sudden change of layer saturation to the one direction either cubic (Ic) or hexagonal (Ih). Thus, on the formation of each interface, we observe the initial halting phenomena where both the forms of ice (Ic and Ih) compete with each other. Not only the selected interface, but the phenomena is also true for each layer formation along the simulation trajectory. This suggests that during basal plane growth, formation of each unique layer is occurring separately through a nucleation type mechanism Apart from the stacking fault there occurs an in-layer stacking where a particular layer consists of both cubic and hexagonal ice at lower temperature. The reason for the in-layer stacking is completely energetic where water molecules are unable to cross the barrier to move forward a particular direction either I_c or I_h. Apart from the stacking fault, in layer defects during basal plane growth at lower temperature happens in a directional way.

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Pd-Catalyzed Intramolecular Oxypalladation-Initiated Domino Reactions: Why does Solvent Polarity Control the Regioselectivity?

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Pd-catalyzed intramolecular oxypalladation-initiated cascade of internal alkyne **1** bearing *N*-tosyl tether can give rise to either functionalized benzazepine **2** via 6-*endo-dig* pathway or tetrahydroquinoline scaffold **3** via 5-*exo-dig* pathway. These benzo-fused nitrogen heterocycles are the building blocks of enormous biologically active natural products and synthetic drug molecules. Surprisingly, the outcome of the cascade reactions is found to be solvent-dependant. While 6-*endo-dig* was the exclusive pathway in 1,4-dioxane solvent, both the 5-*exo-dig* and 6-*endo-dig* pathways were found to be parallelly operative in DMSO (Figure 1).[1] In order to understand the molecular role of the solvent in controlling the regioselectivity, we have performed detailed mechanistic study computationally[2] which can be immensely helpful for further reaction design in environmentally green solvent water. Density Functional Theory (DFT) analysis have shown that formation of the σ-vinylpalladium intermediate can be reversible for the 5-*exo-dig* pathway while it is irreversible for the 6-*endo-dig* pathway in 1,4-dioxane. As a result, the 5-*exo-dig* pathway is found to be unproductive in dioxane. The formation of the σ-vinylpalladium intermediate is irreversible for both 5-*exo-dig* and 6-*endo-dig* pathways in DMSO solvent, and, as a result, both pathways are found to be productive in DMSO solvent. Detailed structural analysis by DFT predicted that the replacement of the *N*-tosyl tether by *O*-tether in the alkyne substrate may stabilize the σ-vinylpalladium complex for 6-*endo-dig* pathway in DMSO solvent. As a result, the carbopalladation activation energy difference between the 5-*exo-dig* and 6-*endo-dig* pathways increases from 1.4 kcal/mol in case of *N*-tosyl-tethered substrate to more than 3 times, 4.8 kcal/mol, in *O*-tethered alkyne, and consequently an exclusive formation of isobenzofuranone-fused chromane **3´** from *O*-tethered internal alkyne substrate **1´** is predicted via 5-*exo-dig* pathway. The experimental study confirms the theoretical hypothesis and provides a highly chemodivergent approach for synthesis of biologically significant complex molecule, isobenzofuranone-fused chromane **3´**, in a single synthetic operation at ambient conditions (Figure 1).

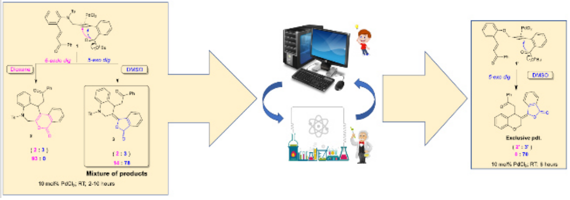

Figure 1. Computational design and experimental verification of the solvent polarity-controlled oxypalladation reactions.

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I-122

Understanding of the Formation and Evolution of Solid Electrolyte Interphase (SEI) at the Calcium Anode Surfaces

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Applications of rechargeable lithium-ion batteries are ubiquitous, but limitations such as raw material scarcity and Li dendrite formation necessitate alternatives to meet modern energy demands. [1,2] Multivalent-metal anode batteries, particularly those using calcium, offer promising advantages like low manufacturing costs, low anodic voltage, fast ion kinetics, and enhanced safety. [3] Nonetheless, the solid electrolyte interphase (SEI) in Ca metal anode batteries (CMABs) hinders ion movement, affecting the reversible Ca deposition at the electrodes. [4] This situation changed in 2016 with the breakthrough work by Ponrouch *et al.*, which demonstrated reversible Ca deposition using only $Ca(BF_4)_2$ salt, not with $Ca(TFSI)_2$. [5] Interestingly, in 2020, they showed reversible Ca deposition with $Ca(TFSI)_2$ but using a passivated electrode. [6] Naturally, these works demand a detailed understanding of (i) *why the reversible Ca deposition is only observed in the presence of* $Ca(BF_4)_2$ *salt but not with the* $Ca(TFSI)_2$ *salt?, (ii) why the* $Ca(TFSI)_2$ *salt showed reversible Ca deposition in the presence of a passivated electrode*?, (iii) *what are the differences between SEIs obtained in* $Ca(BF_4)_2$ *and* $Ca(TFSI)_2$ *salt systems*?, and (iv) *why only some SEIs are permeable to Ca ions*?

To address these questions, we conducted large-scale *ab initio* simulations to study the formation and evolution of SEI at a CMA surface under different electrolytes and temperatures for up to 100 picoseconds. Our findings demonstrate that the $Ca(BF_4)_2$ salt exhibits exceptional stability. On the other hand, $Ca(TFSI)_2$ salt is reductive in nature. Surprisingly, the significant stability of the $Ca(TFSI)_2$ salt is achieved in the presence of a passivated CMA. The demonstrated stability of $Ca(BF_4)_2$ and $Ca(TFSI)_2$ (with the passivated CMA) suggests their potential for participation in redox reactions during charge-discharge cycles, enabling reversible Ca deposition. Furthermore, we found that SEIs formed in the $Ca(BF_4)_2$ system, enriched with organic compounds, are more permeable to Ca than the inorganic-rich SEIs in the $Ca(TFSI)_2$ system. These analyses address the above questions. Overall, the current study provides valuable insights into the complex mechanisms underlying the formation and evolution of SEI on a CMA, which could facilitate the design of new electrolytes to improve the performance and longevity of CMABs. More details are given in the poster.

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I-123

F, B, N-Doped Defective Carbon As Metal-Free Electrocatalyst: Synergistic Effect Augmented Electrochemical Ammonia Synthesis

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Ammonia (NH_3) is crucial in the agricultural industry, serving as a key component in the production of various synthetic materials. Traditionally, the Haber-Bosch process, which converts atmospheric nitrogen (N_2) and hydrogen (H_2) from natural gas into ammonia using iron-based catalysts, requires high pressures and temperatures.[1] Despite its efficiency, this method is energy-intensive and accounts for about 1.5% of global energy consumption, significantly contributing to CO_2 emissions [1] As an alternative, the electrochemical nitrogen reduction reaction (NRR) offers a promising solution by enabling ammonia production under ambient conditions using renewable electricity, with water as the hydrogen source. The metal-free carbonaceous material incorporating heteroatoms and defects presents a promising avenue for electrocatalysts for green ammonia production, offering a sustainable and efficient alternative to traditional metal-based catalysts. Their abundance, cost-effectiveness, and tunable properties make them ideal candidates for electrochemical nitrogen reduction reactions (NRR). In this study, we synthesize a defective N-doped carbon material with boron and fluorine as secondary dopants (FBDG). Boron, being electron deficient, serves as the primary active center, while the carbon atoms adjacent to fluorine acquire a partially positive charge, creating additional active sites for nitrogen adsorption. The synergistic effect of three heteroatoms and defects in the catalyst enhances electron-donor behavior, improving π bonding within the carbon framework and facilitating the electron transfer processes during NRR, resulting in a Faradaic efficiency of 38.1 %. Theoretical calculation of charge density distribution reveals that FBDG possesses sufficient charge density to reduce nitrogen at a low overpotential. The electrocatalyst follows an alternating free energy pathway with a minimal limiting potential. This study elucidates the impact of different heteroatoms in the structure of carbon material and their influence on NRR activity and kinetics.

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I-124

Computational Insights into the Mechanism of Redox-Neutral Decarboxylative Cross-Coupling of Oxamates with Arylbromides

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The formation of an amide bond can be considered as an important transformation in synthetic organic chemistry owing to its presence in proteins, and bioactive molecules like natural products, and pharmaceuticals.[1] Visible light photocatalysis integrated with metal catalysis has opened new avenues in the domain of cross-coupling reactions to form amide bonds.[2] Recently, Reddy and coworkers achieved cross-coupling of cesium oxamates with aryl bromides to form amides employing dual nickel-photoredox catalysis as shown in Figure 1(a).[3] We carried out a detailed mechanistic study using Density Functional Theory (DFT) using oxamate anion (**1a′**) and arylbromide (**2a**) as the substrates. Our studies suggested that the most probable mechanism follows the pathway as shown in Figure 1(b). The major steps involved are as follows: Excitation of the photocatalyst, single electron transfer (SET-1), radical addition to Ni^0, oxidative addition, and reductive elimination. An alternative possibility where the initial step is an oxidative addition step followed by a radical addition step was found to be higher in energy compared to that of the given pathway.

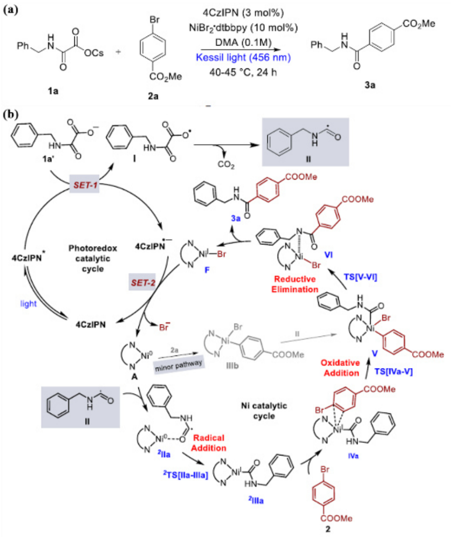

Figure 1. (a) Redox-Neutral Decarboxylative Cross-Coupling of Oxamates with Aryl Bromides. (b) The proposed mechanism for the reaction.

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I-125

DFT Studies on Regioselective 1,2-Alkylboration of Benzylidenecyclopropanes

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The cyclopropyl ring is a crucial component of many preclinical medications,[1] and it is one of the ring systems commonly employed in the production and development of pharmaceuticals. In addition, because of their reactivity, stability, and ease of handling, the organoboronic acid group and its derivatives hold a broad variety of uses in the drug development process.[2] Due to the high strain (38.8 kcal/mol) and simultaneous existence of both cyclopropane and exocyclic double bond, functionalisation of C−C π bond of benzylidene cyclopropanes maintaining the cyclopropyl group is essentially a less explored area. Recently, we worked on the mechanistic studies of copper catalysed regioselective alkylboration of alkylidene cyclopropanes (Figure 1a).[3] Our computational studies involving Density Functional Theory (DFT) calculations suggest that the reaction proceeds via a migratory insertion of alkene followed by a nucleophilic attack of the alkyl halide with C-C bond formation as the rate limiting step and that S_N2-type mechanism is energetically favourable as compared to the radical mechanism (Figure 1b). Alternate pathways and origin of regioselectivity for the product formation were also explored.

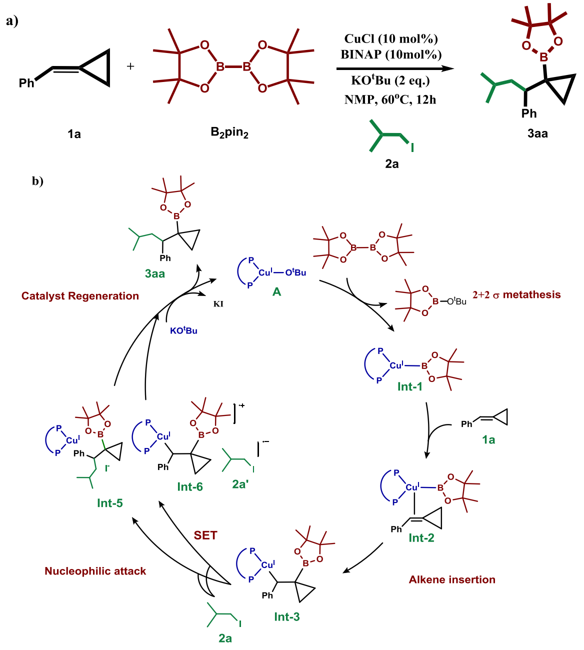

Figure 1: a) Copper catalysed regioselective alkylboration of benzylidene cyclopropanes b) Proposed catalytic cycle

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I-126

Theoretical Study of Hydroxyl Radical Initiated Oxidation Reaction for a Series of Expoxybutane Isomers

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Epoxides are a class of compounds known as oxygenated volatile organic compounds (OVOCs) that are released into the atmosphere from a variety of sources and can have a substantial negative influence on the environment and human health [1,2]. In this work, we have computationally investigated the mechanism, thermodynamics, and reaction kinetics related to the OH radicals' hydrogen abstraction processes of cis-2,3-epoxybutane, trans-2,3-epoxybutane, and 1,2-epoxybutane. Figure 1 displays the reaction schematics and thermochemistry for all the hydrogen abstraction channels. Additionally, potential energy diagrams, including all the species, were constructed at the CCSD(T)/aug-cc-pVTZ//M06-2X/cc-pVTZ theoretical level. The Rice-Ramsperger-Kassel-Marcus-Master Equation (RRKM-ME) adjusted by Eckart tunneling was used to calculate the rate coefficients for every feasible channel within the 200–350 K temperature range and 1 atm pressure, shown in Table 1 [3]. Degradation studies of product radicals indicate that they can lead to the formation of several hazardous end products, including Grade 1 and Grade 2 carcinogens, as classified by the World Health Organization (WHO) [4].

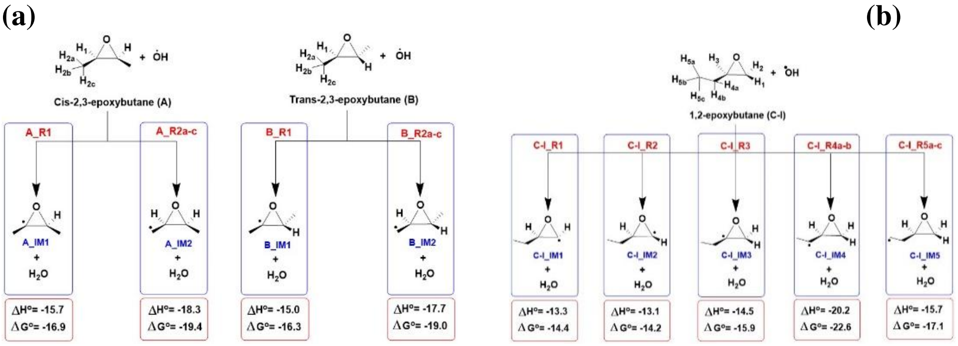

Figure 1. Schematic representation of the reaction pathways and thermochemistry of (a) cis-2,3-epoxybutane (A) and trans-2,3-epoxybutane (B) with OH radicals, and (b) 1,2-epoxybutane (C) with OH radicals.

Table 1. The overall rate coefficients (in cm^3 $molecule^{-1}$ s^{-1}) of cis-2,3-epoxybutane (A), trans-2,3-epoxybutane (B), and 1,2-epoxybutane (C) with OH radicals within the temperature range of 200–350 K.

Compound	**Temperature**						
	200 K	**230 K**	**260 K**	**298 K**	**320 K**	**350 K**	**Experimental at 298 K** [5]
A	19.6×10^{-12}	3.15×10^{-12}	0.93×10^{-12}	0.32×10^{-12}	0.20×10^{-12}	0.11×10^{-12}	$(1.50 \pm 0.28) \times 10^{-12}$
B	16.6×10^{-12}	2.96×10^{-12}	0.93×10^{-12}	0.33×10^{-12}	0.21×10^{-12}	0.12×10^{-12}	$(1.81 \pm 0.33) \times 10^{-12}$
C	56.0×10^{-12}	8.87×10^{-12}	2.32×10^{-12}	0.66×10^{-12}	0.38×10^{-12}	0.23×10^{-12}	$(1.98 \pm 0.29) \times 10^{-12}$

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I-127

Superoxide to Peroxide Interconversion in Ni-TMC Complexes: The Significance of Structure and Spin States

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A deeper comprehension of the characteristics of metal-superoxide and metal-peroxide chemical species is very crucial, considering their pivotal functions in oxygen transport, enzymatic activation, and catalytic oxygenations. O_2 activation is mediated by the interconversion between superoxide and peroxide species. Even though there are multiple studies on metal-superoxide and -peroxide intermediates, robust examples of their synthetic interconversion processes are scarce. For instance, Ni-superoxide/peroxide complexes have been characterized with N-Tetramethylated Cyclam (TMC) ligands with different ring sizes, i.e., Nickel(II)-superoxide complex is characterized with 14-TMC while Nickel(III)-peroxide complex with 12-TMC. Later, both complexes were obtained with 13-TMC ligand by employing different bases; interestingly, no evidence of interconversion between them was identified. What are the factors influencing these processes and why is this preference? We attempted a computational analysis of this issue. 2-dimensional potential energy scan is performed on the 12-TMC, 13-TMC, and 14-TMC systems to identify the reaction path connecting superoxide and peroxide species. We also performed charge analysis, spin population analysis, and transition state optimizations in order to get a clear picture of the interconversion process. The superoxide-peroxide interconversion process appears to be bound by their propensity for distinct structural features and spin states as depicted in Figure 1.

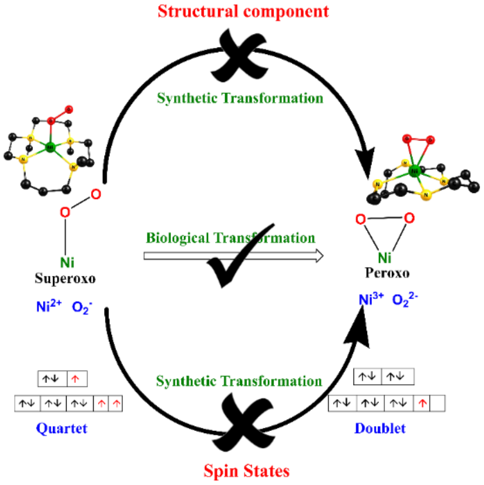

Figure 1. Superoxide – Peroxide interconversion in Ni-TMC system is controlled by structural factor and spin states

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I-128

Unveiling The Novel Mechanistic Insights Into Zinc Catalyzed Sonogashira Cross - Coupling Reaction: A DFT Study

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Sonogashira coupling reactions are considered to be one of the most widely employed transition metal-catalyzed coupling reactions for the synthesis of carbon-carbon bonds. Among the multifarious carbon-carbon bond-forming reactions, those that involve the formation of aryl acetylenes have gained considerable attention in recent times. These reactions are deemed to be versatile tools for the fabrication of molecules having biological and pharmaceutical importance. The high cost, low abundance, and toxicity created a strong demand to search for an alternative to the traditional palladium metal catalyst. Zinc-catalyzed cross-coupling reactions have gathered momentum nowadays owing to the cost-effective and eco-friendly properties of zinc metal. In this presentation, we discuss a detailed quantum chemical study of the Zn (II) catalyzed Sonogashira coupling reaction between aryl halides and terminal alkynes employing DMEDA (*Dimethyl ethelene diamine*) as ligand. All calculations discussed in this presentation are performed at the Density Functional Theory (DFT) level, using the hybrid Becke3LYP functional. We have identified that the active catalyst species is a base-coordinated neutral 4-coordinate DMEDA Zn (II)-alkyne complex. The proposed mechanism proceeds through a concerted oxidative addition-reductive elimination pathway, which involves a single transition state. This is owing to the ease of reductive elimination involving the coupling of Csp^2-Csp carbon atoms and the less stable Zn (IV) intermediate. This shows that the mechanism of Zinc-catalyzed Sonogashira coupling reactions is quite different from those catalyzed by palladium. Furthermore, our study revealed an alternative mechanistic route to Zn-catalyzed Sonogahira coupling reaction, which was expected to proceed via an initial oxidative addition pathway. The activation barrier 31.0 kcal/mol concords well with the experimental temperature requirement (125°C).The complete catalytic cycle for the Zn-catalysed Sonogashira coupling is shown in Figure 1. This work elucidates the relevance of a combined theoretical and experimental approach for rationally improving the cross-coupling reaction mechanisms.

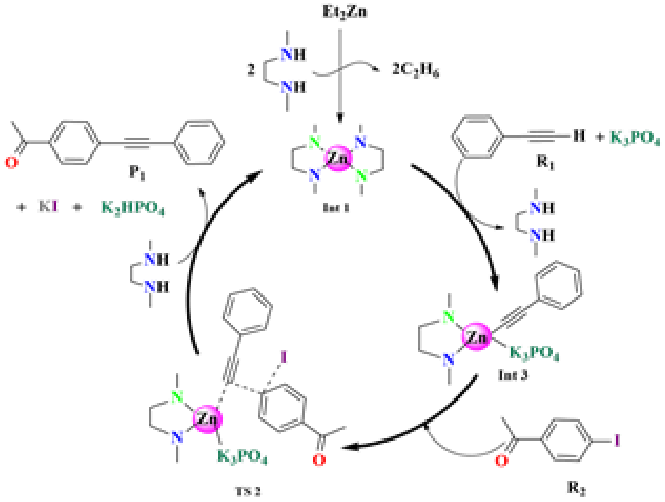

Figure 1.The complete catalytic cycle for Zn(II) catalyzed Sonogashira coupling reaction investigated using DFT/B3LYP-D3/CPCM level of theory.

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I-129

Enhancing Ligand Selectivity in Cross-Coupling Reactions Through Multi-Linear Regression Techniques

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Cross-coupling reactions are a vital method in modern organic synthesis, facilitating the creation of intricate organic compounds by forming carbon bonds with other elements. Despite their utility, selecting the optimal ligand for these reactions remains a significant challenge. This study introduces a multi-linear regression model designed to predict ligand selectivity in cross-coupling reactions. By leveraging a dataset of experimentally derived ligand effects, we pinpoint crucial descriptors influencing ligand performance through Principal Component Analysis (PCA) and develop a predictive model. This model enables the rapid evaluation of potential ligands, enhancing the efficiency of cross-coupling reactions. Consequently, it accelerates the identification of more effective catalysts and improves overall reaction outcomes. The approach not only streamlines the screening process but also contributes to the discovery of novel, efficient catalytic systems for cross-coupling reactions. This advancement holds promise for optimizing reaction conditions and advancing synthetic methodologies in organic chemistry.

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I-130

Understanding the Mechanism of the Acetic Acid Dimerization

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Non-bonded interactions play a critical role in the chemical and biological systems by influencing the structure, properties and functions of the molecules. One such important non-bonded interaction is the hydrogen bonding whose strength vary from 1 to 40 kcal/mol. Carboxylic acid is one of the strong candidates that exhibits hydrogen bonding since it holds a functional group that can act as hydrogen bond donor and acceptor simultaneously. In this work, we take acetic acid as a representative to study the non-bonded interactions, namely, hydrogen bonding.

Different experimental techniques like Mass spectroscopy, Infrared spectroscopy, Raman spectroscopy and Electron diffraction have been used to investigate the possible structures of acetic acid in different phases, viz, solid, liquid and vapour. Crystalline acetic acid is composed of linear chains of hydrogen-bonded molecules. While in the vapour phase, acetic acid exists as a mixture of two species - monomers and dimers, at temperatures above 150 °C. The dimer formed by hydrogen-bonding is known to have a planar ring structure of C_{2h} symmetry from electron diffraction studies; and so it is called a cyclic dimer. The structure of acetic acid in liquid phase is more complex. Some studies have suggested that liquid acetic acid primarily consists of cyclic dimers, while some others have suggested that the main structural patterns in liquid acetic acid are linear chains similar to those found in the solid phase [1]. Taking into account the fact that acetic acid forms a cyclic dimer both in vapour phase and liquid phase, we have aimed to explore the mechanism of formation of the cyclic dimer of acetic acid using computational techniques like 1D (one-dimensional) scanning and 2D (two-dimensional) scanning with the help of Density Functional Theory (DFT). 1D scan was performed taking the distance between two carbonyl carbon atoms of the acetic acid molecules as the reaction co-ordinate. 2D scan was done by taking 2 distances, that is, the distances between carbonyl oxygen of one acetic acid and hydroxyl hydrogen of other acetic acid as the 2 reaction co-ordinates. In addition to this NEB-TS calculation was done to find the minimum energy path. Our analysis shows that dimensionality plays an important role in determining the mechanism of formation of hydrogen bonds in the acetic acid dimerization. Our study shows that the cyclic dimer is stable not only due to the intermolecular hydrogen bonding but also because of the resonance stabilization arising from the intermolecular proton shuttling.

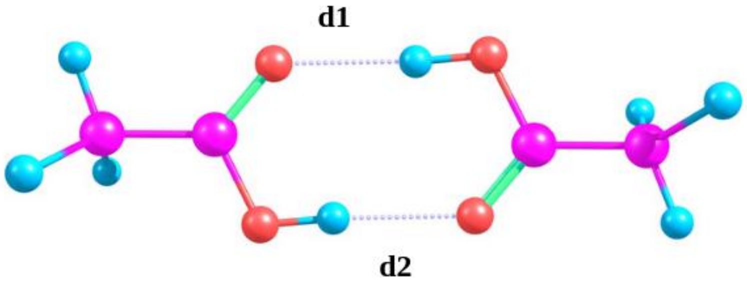

Figure 1. Structure of cyclic dimer of Acetic acid.

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I-131

A Detailed Computational Investigation into the Mechanism of Iron Iodine Catalyzed Ortoleva King Type Reaction

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Imidazo [1,2-α] Pyridines represent a pivotal class of compounds in pharmaceutical research, recognized for their extensive range of biological activities, including potent anti-tumor and anti-cancer properties. This study provides a comprehensive quantum chemical investigation into the mechanism of iron/iodine-catalyzed Ortoleva-King protocol, which offers a highly efficient route for the synthesis of these valuable fused heterocycles. Utilizing a cost-effective and readily available catalytic system comprising $FeCl_3 \cdot 6H_2O$ and molecular iodine, this methodology enables the synthesis of various Imidazo[1,2-α] Pyridine derivatives with impressive yields. The reaction, notable for being both ligand-free and base-free, employs chlorobenzene as the solvent. All calculations were performed using Density Functional Theory (DFT) Level at the hybrid Becke3LYP functional, providing a rigorous theoretical framework. The active catalytic species were identified and the energy pathway was calculated. The proposed reaction mechanism involves a four-step pathway involving: Initiation by activation of the methyl group via molecular iodine, followed by nucleophilic substitution of iodine by aminopyridine, cyclization to form the imidazo moiety, and concluding with dehydration to yield the final imidazo[1,2-α] pyridine product. This work makes a significant contribution to the field by presenting an accessible and scalable method for synthesizing biologically important Imidazo[1,2-α] pyridines, with promising implications for drug discovery and development. Th e work also elucidates the importance of a theoretical and experimental approach for designing efficient reaction mechanisms in the field of organic synthesis reactions.

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I-132

A Theoretical Investigation Into The Mechanism Of The Zinc Catalysed Clauson-Kaas Reaction

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Pyrroles, five-membered heterocyclic compounds with N as the heteroatom, specifically have an essential role in pharmaceuticals, agrochemicals etc. Recently, Clauson-Kaas reactions are being used as a method for synthesising N- substituted pyrroles using various catalysts. Lately, the role of Zinc as a catalyst is widely being studied. Even though there have been a lot of experimental studies of Zinc catalysed Clauson-Kaas reactions, its mechanistic pathways are little-known. Herein we have investigated the mechanism of a Zinc triflate catalysed Clauson-Kaas reaction under neat conditions. This method paves a significant way into the synthesis of N-substituted pyrroles by cost effective and eco-friendly pathway. All calculations were performed using Density Functional Theory (DFT) at the hybrid Becke3LYP functional level, providing a rigorous theoretical framework. The Zinc atom was optimised by the LANL2DZ basis set and other atoms by 6-31(+)G d basis set. In the proposed reaction mechanism, Zinc triflate itself acts as the active catalyst. The mechanism suggests the first step being the binding of the active catalyst to the tetrahydrofuran followed by the addition of the primary amine in a nucleophilic manner. This work provides a theoretical insight into the molecular level mechanism of Zinc catalysed Clauson- Kaas reaction, and helps in designing much more suitable catalysts and reaction conditions for future experiments.

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I-133

Electrocatalytic Mechanisms of the Single Mo Atom on the Holey Graphene for Nitrogen Reduction Reaction Using Constant Potential Ab Inito Molecular Dynamics

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Electrocatalytic nitrogen reduction reaction (eNRR) is an important process, capable of transforming atmospheric nitrogen (N_2) into ammonia (NH_3) at ambient reaction conditions. However, ammonia synthesis heavily depends on the Haber-Bosch process and requires high temperature and pressure. Other challenges such as hydrogen evolution reaction (HER) which is a competitive reaction with NRR lead to lower NH_3 selectivity. To tackle these issues, we theoretically studied the experimentally synthesised single Mo atom anchored on N-doped graphene (Mo-N_3) and holey graphene (Mo-N_3-$2V_c$) catalyst at applied potential -0.25 V and -0.05 V vs RHE, respectively [1,2]. Furthermore, to get computational insight into NRR catalytic activity, we used a combined approach of the computational hydrogen electrode model (CHE) and the capacitor model to calculate the potential-dependent activation free energy barrier of the potential determining step (PDS) in the presence of hybrid solvation model [3]. Our study showed that Mo-N_3-$2V_c$ is an efficient catalyst with a limiting potential of 0.197 V (Figure 1(a)) with a reaction barrier is 0.542 eV (*N_2 to *NNH), at an applied potential. We employed the constant potential ab initio molecular dynamic simulation (CP-AIMD) approach to maintain the reaction potential during the simulation, to calculate the activation barrier at a potential of -0.05 V through the blue moon sampling method. Our systematic study shows that the barrier calculated from the CP-AIMD (Figure 1(b)) was relatively lower than the barrier calculated from the capacitor model. Overall, this investigation shows the effect of applied potential on the reaction barrier with and without changing the background electrons.

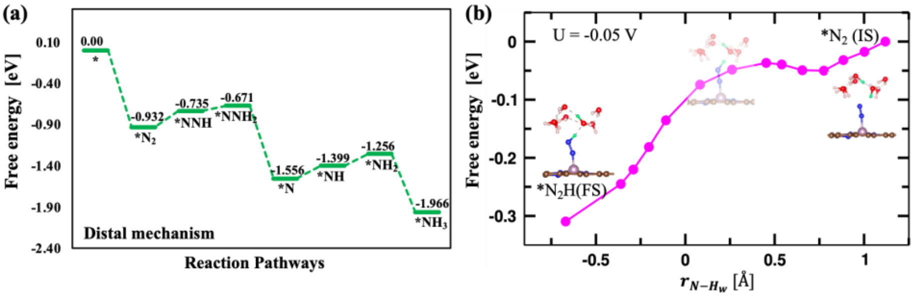

Figure 1. (a) The Gibbs free energy diagram of Mo on the holey graphene (CHE) (b) The free energy diagram for the PDS on Mo-N_3-$2V_c$ at -0.05 V (CP-AIMD).

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I-134

A Computational Investigation into the Molecular mechanism of Ligand Assisted Manganese Catalyzed Ullmann Cross Coupling Reaction

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Ullmann coupling reactions are one of the most widely employed transition metal-catalyzed coupling reactions for C-O bond coupling. These reactions have great significance and extensive applications in the pharmaceutical and biological fields. The high cost, low abundance, and toxicity created a strong demand to search for an alternative to the traditional copper metal catalyst. Manganese-catalyzed cross-coupling reactions have been recently relevant because of their sustainable and eco-friendly properties. In this work, we discuss a detailed Density Functional Theory (DFT) study of the Mn (II) catalyzed Ullmann coupling reaction between aryl halides and phenols by employing DMEDA (Dimethyl ethylene diamine) as ligands. All calculations discussed in the work are performed at the DFT level, using the hybrid B3LYP functional augmented with CPCM solvation model using acetonitrile as the solvent. The Mn and I atoms are described using (LANL2DZ) and the C, H, N and O atoms were described by a 6-31+G(d) basis set. We have identified that the active catalyst species is a three-coordinated DMEDA ligated Mn (II)-phenoxide complex. The proposed mechanism proceeds via a σ bond metathesis, involving a single transition state. The activation barrier 32.4 kcal/mol concords well with the experimental temperature requirement (110° C). This study primarily investigates the relevance of enhancing the mechanisms of cross-coupling reactions through both theoretical and experimental methodologies [1].

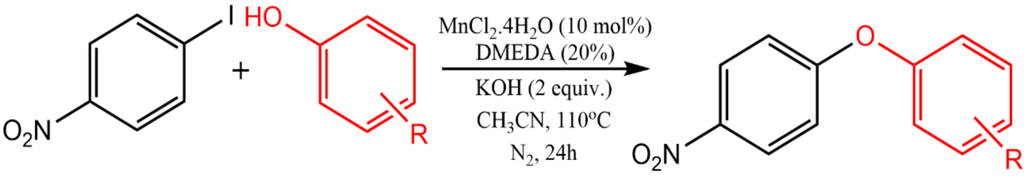

Figure 1. The model reaction for the ligand-assisted Mn-catalyzed etherification reaction

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I-135

Computational Investigations on the Photo-isomerization of Nitrones and Thermal Isomerization of the Photoproduct Oxaziridine

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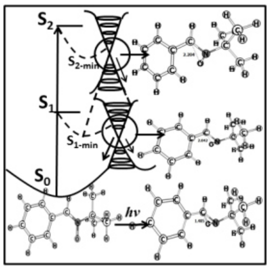
Nitrones are known to be important pharmacological agents. Both cyclic and acyclic nitrones are known to be photosensitive in nature. Experimental studies on their photo-isomerizations have been reported since last six decades. However, the exact mechanisms of these processes were not known till recent times. The reaction pathways involved in these photochemical reactions have been explored through computational studies by our group in the last one decade. The studied systems include different types of acyclic and cyclic nitrones, such as the chemopreventive retinyl nitrones (and their model compounds), the fluorescent naphthyl nitrones, α-styryl N-methyl nitrones, spin trap agents like DMPO, TMPIO, PBN and so on [1-4]. Studies on few other types of nitrones having high biological importance are going on at present. High-level quantum mechanical studies have revealed the photochemical pathways of these nitrones. Photo-excitations of these molecules found to undergo non-radiative decay through conical intersection channels involving the S_0, S_1 and higher excited singlet states. The photo-isomerization primarily leads to the photoproduct oxaziridine which has a terminally kinked CNO moiety. Depending on the nature of the substituents (on N and C), the oxaziridine formed can be stable or may lead to amides. The *N*-alkyl α-phenyl nitrones are well-known for their pharmacological importance. One of the most important nitrones of this category, PBN has been extensively studied under photo-irradiation in past. In recent times, the isomerization pathways of this spin trap nitrone have been thoroughly studied by us (Figure below) to understand the effect of the phenyl group [1]. In addition to its photo-isomerization, the thermal nitrogen inversion mechanism of oxaziridine (the photoproduct) was explored which can be of high significance to the organic chemists. Currently, our group is involved in understanding the influence of the electron-donating /withdrawing substituents (present on the α-phenyl ring) on this photo-isomerization and the chiral nitrogen inversion mechanisms.



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I-136

Role of Ring Strain and Unsaturation in the Gas-Phase Reactivity of Cyclic Compounds with Atmospheric Oxidants

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Introduction

Volatile Organic Compounds (VOCs) in the atmosphere cause major environmental impacts such as photochemical smog, global warming, indoor human exposure and work environments [1]. The OH radical oxidation is the major tropospheric removal channel and decides the fate of the majority of the VOCs. Ozone reaction is also important for unsaturated VOCs. In this work, we have experimentally determined the OH and O_3 rate coefficient of cyclic compounds with different structural features. Structure reactivity is correlated by mapping the potential energy surfaces of these reactions and locating the minimum energy pathway among the available sites.

Results and discussion

OH and O_3 oxidation reaction was experimentally studied for 1-methyl cyclopentene and 1,3-dioxolane and results were compared with 3-membered cyclic ether epichlorohydrin. For the ozone reaction, reactivity for 1-methyl cyclopentene was found to be the highest as expected. Surprisingly, 1,3-dioxolane (Fig. 1) was found to react with ozone via H-abstraction pathway. Theoretical calculation suggested the stabilisation of transition state by the inductive effect of two oxygen atoms in the above reaction. For the OH radical reaction too, 1-methylcyclopentene was found to have the maximum reactivity. The room temperature OH rate coefficients of epichlorohydrin, 1,3-dioxolane, 1-methyl cyclopentene experimentally obtained by studying the gas-phase kinetics of their reactions with OH radical were found to be (cm^3 $molecule^{-1}$ s^{-1}) $(3.81 \pm 0.33) \times 10^{-13}$; $(1.27 \pm 0.03) \times 10^{-11}$; $(1.17 \pm 0.24) \times 10^{-10}$ respectively. The reactivity of epichlorohydrin was found to be two order of magnitude greater than the 1,3-dioxolane. To understand the reason behind the difference in reactivity, theoretical mapping of the PES was done at QCISD(T)/6-311++G(d,p) level. Considering the minimum energy pathways of all the reactions, the activation energy was found to be 4.3 kcal/mol for epichlorohydrin while it came out to be 3.5 kcal/mol for 1,3-dioxolane. The higher *s* character of C-H bonds in 3-memrbered ring led to increased bond strength and in turn lower reactivity. The minimum energy pathway for the reaction of 1-methyl cyclopentene with OH radical was found to involve a pre-reactive addition complex, suggesting the superiority of addition channel over the abstraction channel in VOC+OH reaction.

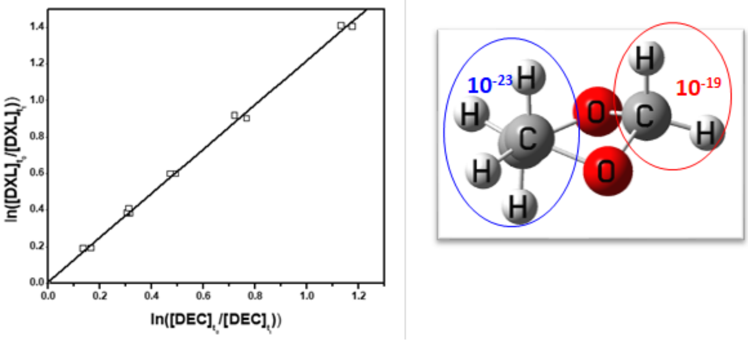

Figure 1. Experimental plot of rate coefficient of 1,3-dioxolane+ozone reaction (left), theoretical rate coefficient of different set of abstraction sites calculated sing TST with Wigner correction (right)

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J-121

Theoretical insights into ellagic acid-induced destabilization of α–Syn oligomers in Parkinson's disease

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The intracellular neuronal aggregates comprising α–Synuclein (α–Syn) protein known as Lewy bodies and Lewy neurites are the key hallmarks of Parkinson's disease (PD) [1a]. The destabilization of disease-relevant α–Syn fibrils is considered a key therapeutic approach against PD [1b]. Ellagic acid (EA), a natural polyphenolic compound, is experimentally proven as a potential candidate that reverses the α–Syn fibrillization [2]. Continuing with our efforts on illuminating the inhibitory mechanism of various inhibitors against Aβ aggregation and protofibril destabilization [3], molecular dynamics (MD) simulations have been performed in this work to unveil the destabilization mechanism of EA on α–Syn oligomers (Fig.1) [4]. EA interacted primarily with the non-amyloid-β component (NAC) of α–Syn oligomer, disrupting its β-sheet content with a concomitant increase in the coil content. The E46–K80 salt bridge, critical for the stability of Greek-key-like α–Syn fibril, was disrupted by EA. The computational studies exploring the effect of small molecules on the destabilization of oligomers of varying sizes are worthy for gaining insights into the discovery of new inhibitors of α–Syn aggregation and protofibril destabilization in PD.

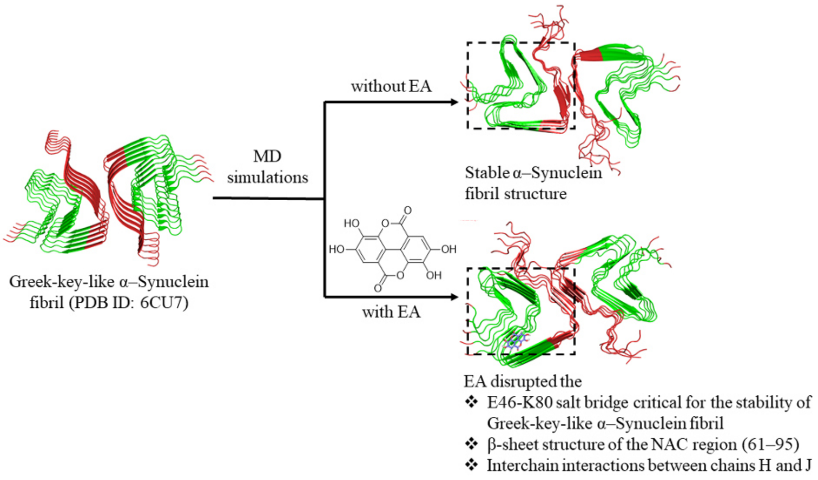

Fig. 1: EA-induced destabilization of α–Syn oligomers.

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J-122

Comparative Insights into the Potential of Two Carotenoids, Zeaxanthin and Peridinin, for Fibril Inhibition in $A\beta_{17-42}$ Oligomer

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In neurodegenerative diseases like Alzheimer's, the quest for agents that can destabilise the AB fibrils and prevent organisation into stable sheets leading to plaques have led us to phytochemicals, owing to their non-toxicity and bioavailability. Recently, carotenoids have been identified as potential candidates against such neurodegenerative diseases [1]. In this regard, we have investigated the potential effects of two carotenoids in aqueous environment of $A\beta_{17-42}$ oligomer. Peridinin is an apocarotenoid pigment that is used by organisms like dinoflagellates for photosynthesis while zeaxanthin is a xanthophyll carotenoid found in orange pepper, saffron, paprika, goji berries. The structures of the ligand molecules are obtained from PubChem and the protein PDB (2beg.pdb) is obtained from RCSB (Figure 1(a)), as has been used in literature[2]. Desmond, Schrödinger LLC was used to perform molecular dynamic simulations for 100 ns. The receptor–ligand complex was pre-processed by using Protein Preparation Wizard of Maestro, which included complex optimization and minimization. In the simulation, the OPLS 2005 force field with TIP3P solvent model was used. The NPT ensemble with 310 K temperature and 1 atm pressure was chosen for the entire simulation. The trajectories were saved for examination after every 100 ps, and the simulation's stability was verified by comparing the protein and ligand's root mean square deviation (RMSD) over time. The results in Figure 1 (b) and (c) demonstrate protein-ligand contacts over the entire course of the simulation for both the candidates, with peridinin having stronger binding as is evidenced from the initial docking results as well (-5.6 kcal/mol for peridinin, -2.1 kcal/mol for zeaxanthin). Peridinin, in comparison with zeaxanthin, is able to destabilise overall secondary structure propagation, while the former is only able to prevent helix formation and has negligible effect on beta-strand distribution. These initial insights prompt further investigations into the potential of structural tuning of phytochemicals for fibril inhibition.

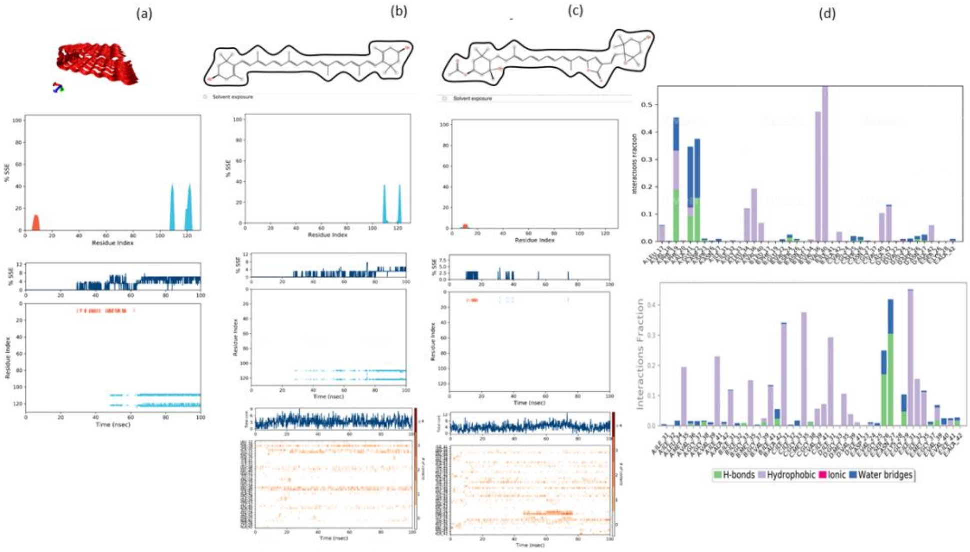

Figure 1: (a) Control run with 2beg.pdb in water showing initial secondary structure timeline (b) Zeaxanthin's effect on secondary structure and protein-ligand contact timelines c) Peridinin's effect on secondary structure and protein-ligand contact timeline d) Protein-ligand Interaction type distribution in zeaxanthin (top) and peridinin (bottom)

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J-123

Conformational Properties of Poly(A)-Binding Protein Complexed with Poly(A) RNA

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Microscopic understanding of protein−RNA interactions is important for different biological activities, such as RNA transport, translation, splicing, silencing, etc [1]. RNA-binding proteins (RBPs) containing multiple RNA recognition motifs (RRMs) are expected to interact differently with the RNA [2]. Polyadenine (Poly(A)) binding proteins (PABPs) make up a class of regulatory proteins that play critical roles in protecting the poly(A) tails of cellular *m*RNAs from nuclease degradation. In this work, we performed molecular dynamics (MD) simulations using the GROMACS computational package [3] to investigate the conformational modifications of human PABP protein and poly(A) RNA that occur during complexation [4]. It has been demonstrated that the intermediate linker domain of the protein transforms from a disordered coil-like structure to a helical form during the recognition process, leading to the formation of the complex. On the other hand, disordered collapsed coil-like RNA on complexation has been found to transform into a rigid extended conformation. Importantly, the binding free energy calculation using the Molecular Mechanics Poisson−Boltzmann Surface Area (MMPBSA) [5] method showed that the thermodynamic stability of the complex is primarily guided by favorable hydrophobic interactions between the protein and the RNA.

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J-124

Exploring the Properties of Aβ Oligomers in Aqueous Ammonium-Based Ionic Liquid Solutions

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Aggregates of amyloid-β (Aβ) peptides are markers of Alzheimer's disease (AD), a condition characterized by irreversible memory loss and cognitive decline in adults. Studies involving Aβ monomers suggest the formation of soluble toxic oligomers that eventually develop into insoluble fibrils [1]. Understanding the precise mechanism of hydrophobic collapse leading to Aβ aggregation is crucial for designing drugs and treating AD [2]. Recently, the impact of electrostatic interactions in room-temperature ionic liquids (RTILs) on protein amyloidogenesis has garnered special attention [3]. This study uses molecular dynamics simulations to explore how trimethylammonium chloride (TMAC), cholinium chloride (ChoC), and tetrabutylammonium chloride (TBAC) ionic liquids (ILs) affect the conformational stability and association mechanism of aggregation prone Aβ pentamer. These ILs, characterized by varying hydrophilicity/hydrophobicity, exert differential effects on conformatioanl flexibility of Aβ oligomer. Moreover, Mechanistic insights derived from umbrella sampling simulations further elucidate how ILs modulate the association/dissociation of Aβ monomers within oligomeric aggregates. Our findings indicate that compared to pure aqueous medium, the binding of Aβ peptide becomes less favourable in presence of the ILs with binding propensity decreasing from TMAC to TBAC solutions, as evident from Figure 1. Further, energy landscape analysis of Aβ peptide docking to Aβ oligomer reveals multiple low-energy conformations, which are more dispersed in presence of ChoC and TBAC solutions, potentially hindering Aβ prefibril growth.

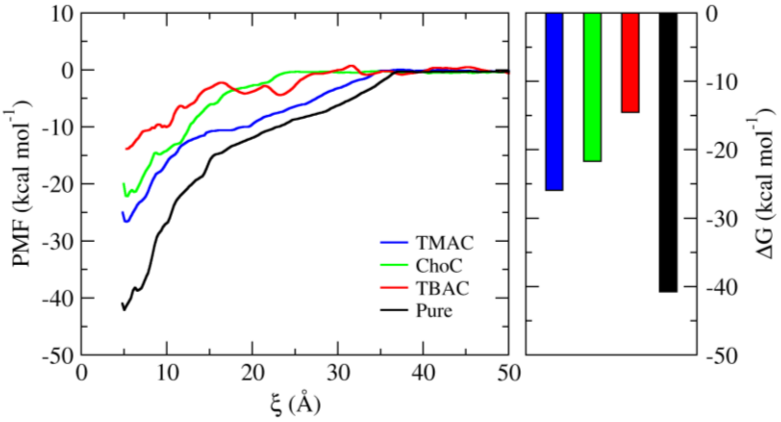

Figure 1. Variation of the potential of mean force (PMF) along the reaction coordinate for Aβ pentamer in different ammonium-based aqueous IL solutions and in pure water. The corresponding free energies of binding (ΔG) of peptide monomer to Aβ pentamer are shown in right panel.

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J-125

Harnessing Quantum Chemical Methods to Unravel the Ethylene Sensing Mechanism in Plant Receptors Amidst Structural Obscurity

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Considering their complexity, it is truly a marvel how living systems can precisely orchestrate their growth, reproductive, and functional processes on cue from certain molecular 'signals'. Fruit ripening is a classic example of this phenomenon. Ripening, a highly intricate process that converts a green, immature fruit into a more palatable one through biochemical changes - such as the accumulation of sugars, flavor and aroma compounds, biosynthesis of pigments in the peel, and softening of fruit tissue - is initiated in response to a single plant hormone: ethylene. The tight association of ethylene with fruit ripening has direct agronomic implications, particularly in the post-harvest storage of fruits [1].

Ethylene elicits its response through the copper-containing transmembrane receptor, Ethylene Response 1 (ETR1). Due to the unavailability of structural information on ETR1, our current understanding of the ethylene sensing mechanism is limited and the copper- receptor, ligand-receptor interactions as well as the roles of specific amino acid residues remain unsolved at large [2]. A detailed understanding of ethylene perception, which is the starting point for understanding the action of ethylene, is crucial for designing effective strategies to manipulate fruit ripening.

The objective of the present work is to decipher the aforementioned unknowns about the nature of ligand-receptor interactions in ETR1. To achieve this, we have employed density functional theory-based methods on hierarchical amino acid models of the ETR1 binding site and systematically investigated the copper and ethylene binding processes. Our analyses shed light on previously unknown aspects, such as the nature of copper coordination before and after ethylene binding, the functional roles of binding site amino acid residues, and the structural and electronic changes following ethylene binding, which together provide a comprehensive description of the characteristics of the ethylene-ETR1 interaction.

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J-127

Anticipating Functional Responses from Protein-DNA Interactions Networks

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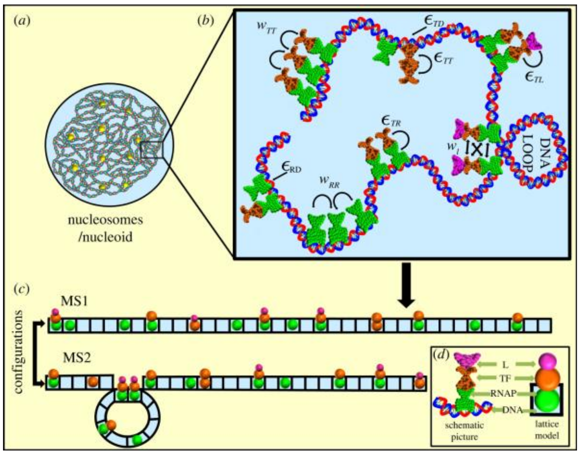
The origin of an ordered genetic response of a complex and noisy biological cell is intimately related to the detailed mechanism of protein-DNA interactions in various gene regulatory systems. However, the quantitative prediction of genetic response and the correlation between the mechanism and the shape of the response curve is poorly understood. Here, we seek to understand the detailed protein-DNA interaction mechanisms observed in gene regulatory networks and anticipate the shape of the functional responses. We show that the shape of the response curves is modified significantly by including layers of biophysical events such as transcription factor (TF) oligomerization, TF-signaling molecule interactions, and DNA looping. To carry out these calculations, we propose system-specific grand canonical partition function-based statistical thermodynamic models and in silico studies of various gene regulatory networks by examining a system containing multiple interacting genes, where we include all the above biophysical events into the model. We validate our predictions against experimental findings for the lac operon system using our proposed models and Grand Canonical Monte Carlo simulations.



(*a*) Schematic view of the complex structure of nucleosomes/nucleoid. (*b*) The zoomed view of a section of nucleosomes/nucleoid. Different types of protein–DNA interactions control the populations of a specific configuration. (*c*) Protein–DNA interactions are modeled as a lattice of possible binding sites that TFs can occupy. Two possible configurations out of an enormous number of microstates are shown for representation. (*d*) A correspondence between the bead and 3-D structures of protein and DNA is shown.

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J-128

Investigation of Natural Compounds as Possible Therapeutic Agents that Inhibit the ODC Enzyme's Carcinogenic Activity.

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The MYC oncogene is known to be targeted by the ornithine decarboxylase enzyme, establishing a link between polyamine metabolism and oncogenesis in both healthy and malignant cells. Many malignancies are linked to ODC activation and increased polyamine activity, and changes in ODC protein levels have a significant impact on cellular activity that inhibits or suppresses tumor cells.[1] This study explores the patterns of inhibition of naturally existing inhibitors and the potency of recently developed natural compounds as inhibitors of the Ornithine decarboxylase enzyme.[2] In this work, approximately 300 natural compounds reported from 51 distinct medicinal plants are screened virtually using pharmacokinetic characteristics tests and molecular docking studies. The high docking score suggests a higher binding affinity between the ODC protein and the organic compound involving strong noncovalent interactions specified for advancement toward discovering a more effective natural inhibitor for the carcinogenic activity of the ODC enzyme. Finding a reversible natural inhibitor to fill in the gaps in cancer prevention caused by the ODC enzyme has been suggested by Molecular Dynamics simulation studies. 9 variations of natural compounds, including flavonoids, terpenoids, alkaloids, and steroid-based compounds, are subjected to simulation studies over 100ns time series. Nevertheless, we have discovered that molecular dynamic simulation studies of specific triterpenoids and natural flavonoids depicted in Figure 1 are superior substitutes and promising treatment options for decreasing ODC enzyme activity.

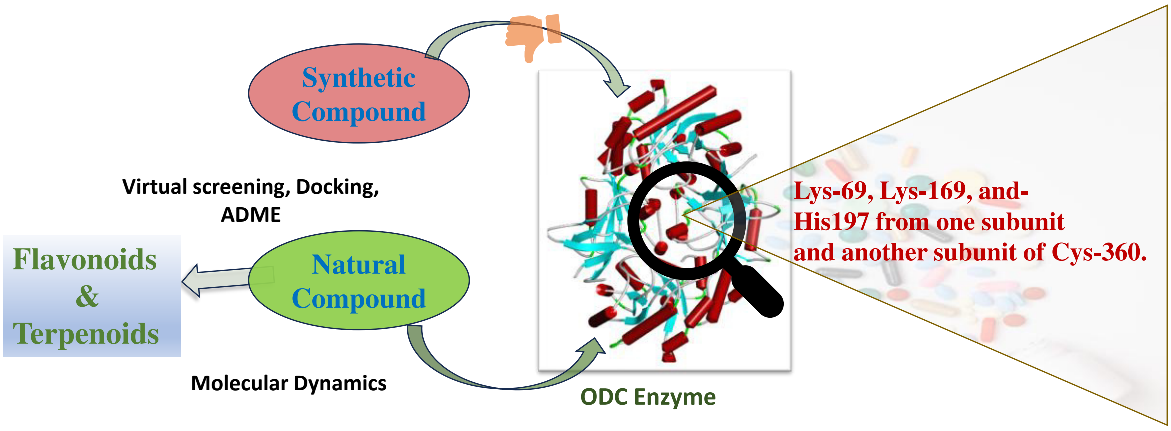

Figure 1: Flavonoids and Terpenoids natural compounds can be potent inhibitors for the Ornithine Decarboxylase enzyme suggested by molecular dynamic Simulation Studies.

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J-129

Interplay between Uranyl ion and fatty acid binding to Human serum albumin: All atom molecular dynamics simulation study

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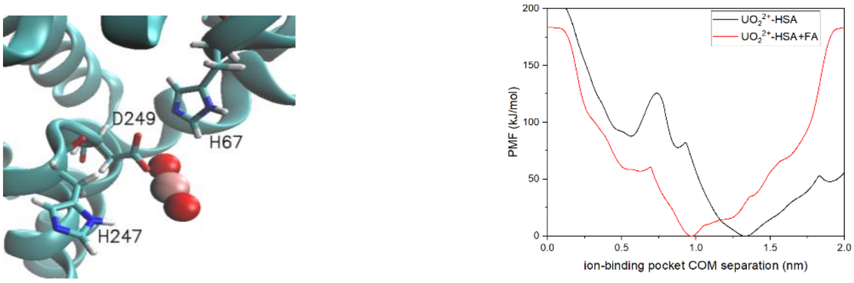
Actinides once internalized, interact with biological ligands (proteins, amino acids, etc.) to mimic natural biological elements (iron, calcium, etc.), although the phenomenon remains obscure. Human serum albumin (HSA), The most abundant plasma protein, is a key player in these interactions. HSA with approximately 55% of total protein in plasma and a concentration of 3.5-5 g/L, possesses multiple binding sites. Uranium is routinely handled in various stages of the nuclear fuel cycle, and its association with HSA has been reported [1]. Investigating the interactions between U(VI) and HSA is of pivotal importance for unravelling the molecular mechanisms of toxicity and the trafficking of uranyl cations in organisms. It is understood that albumin serves as a carrier for several ligands within the living organism. Though interactions of various ligands with albumin are extensively studied, interplay of two ligands is rarely documented. In plasma, HSA transports both fatty acids (FAs) and metal ions. The metal-FA crosstalk is successfully established by using experimental techniques [2]. However, studying dynamic transitions between conformations experimentally remains highly challenging. In present study, all atom molecular dynamics (MD) simulations are employed to understand the interplay of the FA and uranyl ions binding to HSA at the molecular level.

For this, PDB structure of defatted metal free HSA(1AO6), HSA with zinc(5IJF) was taken from RCSB data bank and processed to get all systems at physiological pH. The uranyl ion force field parameters are taken from existing literature and it is docked at zinc binding site (fig 1(a)). All the MD simulations are carried out by applying the CHARMM31 force field parameters in the GROMACS suite of program. The well-tempered meta-dynamics(WT-MtD) simulation is executed using PLUMED plugin to understand binding and unbinding pathways. Hydrogen bonding dynamics analysis reveals the disruption of existing bonds due to fatty acid binding, contrasting with the weakening effect caused by metal binding. Short range Coulomb interactions and PMF profiles from WT-MtD simulations reveals that FAs enhance the UO_2^{2+} ion binding with HAS (fig 1(b)). Uranyl ion introduced at zinc binding site moves away and interacts with residues implicated in calcium binding. Introduction of fatty acid enhances the uranyl-HSA interaction similar to calcium, this is opposed to zinc behaviour as it leaves binding pocket on introduction of FA. The uranyl ion is observed to mimic calcium biological behaviour, further study of uranyl and calcium ions with HSA is planned in future.



(a) (b)

Figure 1.(a) Initial structure of the UO_2^{2+}-HSA (b) PMF profiles for the unbinding transition by employing COM between ion and binding pocket as collective variable

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J-130

Identifying Biochemical Indicators to Detect Critical Transitions in Cdc2-cyclin B/Wee1 System

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The Cdc2-cyclin B/Wee1 kinase system exhibits bistability between alternative steady states, which emerges due to the mutual inhibition between Cdc2-cyclin B and Wee1 kinases, also known as a mutually inhibitory or double-negative feedback loop. The alternative steady states are M phase-like state and G2 arrest-like state, which have implications in the cell cycle progression at the G2 phase in eukaryotic cells. A slight alteration in the feedback strength can drive critical transitions between these contrasting alternative states upon crossing a critical threshold or a tipping point. The phenomenon of critical slowing down (CSD) has been widely used to identify the proximity to a critical transition [1]. However, determining the key variable or species that best signals CSD is a challenging task [2] and holds significance in complex biological processes. Here, we determine the leading variable or observation direction (OD) from the direction of CSD to forewarn abrupt transitions in the Cdc2-cyclin B/Wee1 model system. Figure (1) depicts the mutually inhibitory loop between Cdc2-cyclin B and Wee1 and the inset shows the change in CSD direction near a tipping point. We find that with increasing feedback strength, the Cdc2-cyclin B is the OD. With decreasing feedback strength, both Cdc2-cyclin B and Wee1 can be used as OD. Further, the noise-sensitive direction highlights the impact of external stochasticity in Cdc2-cyclin B and Wee1 directions for increasing and decreasing feedback strength, respectively. We also perform sensitivity analysis that reveals the robustness of the observation direction. Finally, we compare the CSD-based detection of OD with principal component analysis.

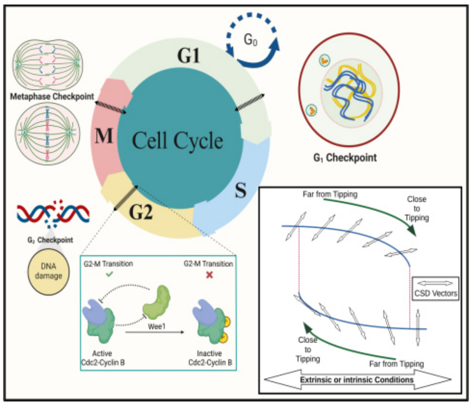

Figure 1. Schematic diagram illustrating key checkpoints in the cell cycle. Each checkpoint regulates proper progression through the cell cycle phases. The inline depiction highlights that the direction of CSD may vary in the vicinity of the tipping threshold.

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J-131

Designing Expanded and Contracted Porphyrin-Azulene based Photosensitizers for Photodynamic Therapy

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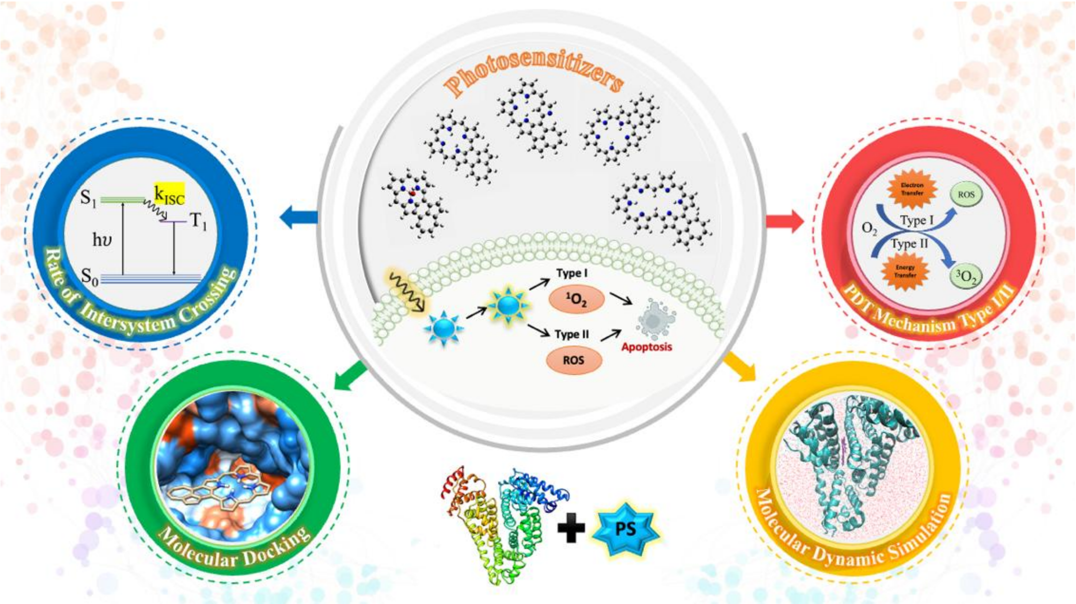
Photodynamic therapy (PDT) is a non-invasive cancer treatment technique with better therapeutic efficacy. A photosensitizer (PS) plays a crucial role in PDT, providing a gateway to enter the biological system without surgery safely. The PS absorbs energy in a biologically safe window and is involved in useful photochemical reactions within the cells to destroy the infected cells without affecting the healthy cells. In our previous work [1], we have already demonstrated their efficacy of absorbing one- and two- photons in a biologically safe window. This study investigates the potential of ten porphyrinoid-azulene based systems devoid of heavy metals as promising photosensitizer candidates to be used in photodynamic therapy (PDT). Through a comprehensive exploration of various photophysical properties, including inter-system crossing, triplet excited state lifetime, and solvation-free energy, employing the state-of-the-art time-dependent density functional theory utilizing B3LYP/6-311+G(d,p) level, we assess their efficacy as photosensitizers in PDT. Furthermore, the interaction of the proposed photosensitizers and Human Serum Albumin, focusing on identifying specific drug binding sites, i.e., Sudlow's site I/II, is explored through molecular docking and molecular dynamics simulations.



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J-132

Unveiling Conotoxin PIXIVA Architecture: A Molecular Dynamics Study

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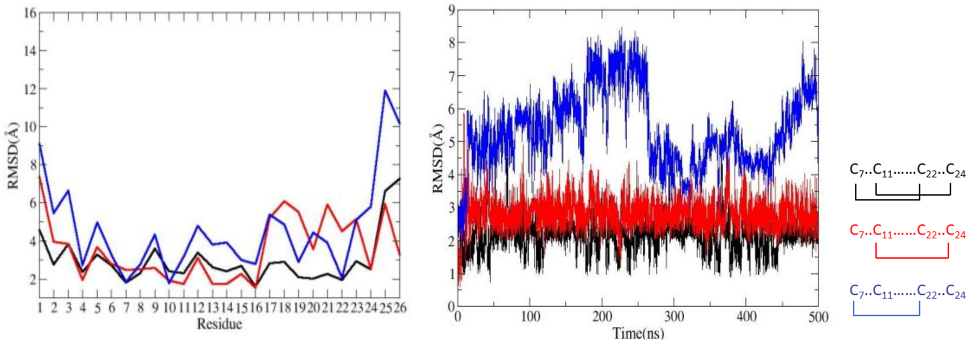
Conotoxins, a diverse collection of peptides discovered in the venom of Conus cone snails, possess remarkable pharmacological properties. They are small peptides stabilized by disulfide bonds and fold into unique three-dimensional structures. Their potential for therapeutic applications in various fields, such as pain management, treatment of neurological disorders, and drug development, has garnered significant attention [1,2]. Known for their high specificity, and potent activity, and most of all, they are non-addictive analgesics used for treating chronic pain, its target includes Ion channels, receptors, GPCRs, etc.



Conotoxin PIXIVA is a J-superfamily conotoxin with 26 residues and 2 disulfide bonds (1-3,2-4) connectivity. It is known to have potent activity in both Nicotinic Acetylcholine Receptor and Voltage-Gated Potassium Channel 1.6 channel. Kv1.6 (IC_{50} = 1.59 μM), neuronal (IC_{50} = 8.7μM for α3β4) and neuromuscular (IC_{50}=0.54 μM for α1β1εδ) subtypes of nicotinic acetylcholine receptor. [3] This work focuses on the structural aspects of the toxin, and the importance of each cysteine linkage as these cysteine linkages in such peptides are often crucially related to their structural integrity and functional potency. In this work, we employed molecular dynamics simulation to study the stability of the conotoxin in water, the system was simulated for 500ns at 300K and the disulfide bonds were broken one at a time to see which disulfide bond contributed more to the stability of the conotoxin.

Based on the data presented in figures (a) and (b), it is evident that the removal of the Cys_{11}-Cys_{24} disulfide bond has had a greater impact on the stability of conotoxin PIXIVA. Figure (b) illustrates that, upon the removal of this disulfide bond, the toxin exhibited the expected free movement. The backbone RMSD graph indicates that the removal of the Cys_7-Cys_{22} disulfide bond did not significantly affect the stability, while the removal of the Cys_{11}-Cys_{24} disulfide bond destabilized the conotoxin's structure. This finding provides valuable insight for our future research, particularly in our study of the conotoxin's binding interaction and selectivity with its target receptor.

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J-133

Membrane Remodelling in Thermal Adaptation of Marine Algae

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Marine macroalgae are diverse photosynthetic organisms, essential for the marine ecosystem. They are environmentally sustainable sources of numerous bioactive compounds having wide industrial applications. Marine algae are exposed to rigorous environmental stress including fluctuations in temperature that significantly affect algal growth and productivity. Alteration in lipid composition and acyl chain unsaturation is a prominent response of algae to temperature stress. By adjusting lipids cells believe to maintain the fluidity or integrity of their cell membranes for optimal functioning in a process called homeoviscous adaptation, but the mechanism is yet not well understood. To study the effect of changes in seawater temperature on the cellular membranes of algae, we employ Molecular Dynamics simulations with all-atom representation. We present the first realistic models of algal thylakoid membranes mimicking the lipid composition of commercially important red algae and explore the temperature-dependent phase behavior of the model membrane at atomistic resolution [1]. The membrane undergoes a gel-to-fluid phase transition over a range of 10°C-40°C temperature (Figure 1). We observed spontaneous phase separation into co-existing domains near the optimal growth temperature (30°C). Our results provide detailed molecular insights into how the adaptive rearrangements of lipid/fatty acid components of algal cellular membranes contribute to the acclimation process, counteracting the effects of temperature. This has implications for developing strategies to enhance the thermal tolerance of algae, which is particularly important in the context of global warming and for sustainable algal cultivation.

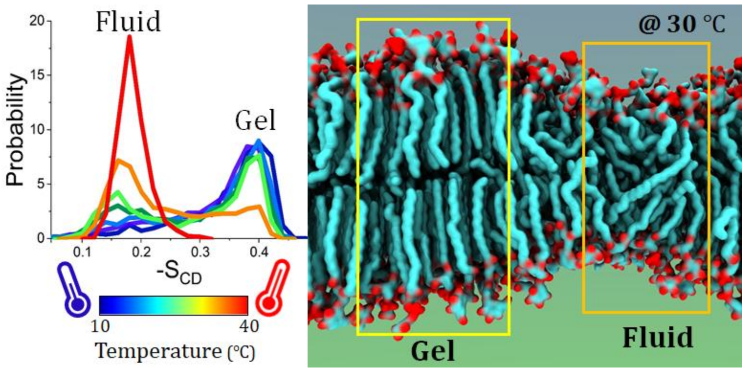

Figure 1. Gel-to-fluid phase transition of thylakoid membrane of algae as a function of temperature.

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J-134

Puckered vs Buckled Phosphorene Monolayers for Sensing COVID-19 Biomarkers A DFT Study

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Globally, COVID-19 caused a potential risk to human health, especially due to incompletely recovered discharged patients based on the RT-PCR results. Owing to the low accuracy of RT-PCR, researchers are seeking to develop 2D materials for sensing COVID-19 biomarkers, which is gaining much attention. In this work, the two pristine phosphorene monolayers (Fig.1.b), namely black (puckered) and blue (buckled), have been chosen for investigating their sensing performance towards COVID-19 biomarkers [1], namely 2-Pentanone, Tetrahydrofuran, benzaldehyde, and 2-Methylpent-2-enal(Fig.1.a) in both vacuum and humid media. The band structure revealed the semiconducting nature of both monolayers. Ab initio molecular dynamics (AIMD) at T=300 K and phonon studies confirm that the monolayers are thermally and dynamically stable [2]. The adsorption energies ranging from **-0.21 to -0.62 eV** exhibit the existence of physisorption between monolayers and biomarkers, and further, Bader charge analysis confirms the presence of weak interactions. Besides the study reveals that the buckled (blue) phase phosphorene exhibits high sensitivity in the range of 92.6% to 99.9% towards sensing biomarkers such as benzaldehyde, 2-Methylpent-2-enal, Tetrahydrofuran, and 2-Pentanone in comparison with the puckered (black) phase phosphorene in the range 0.77% to 74% in vacuum and humid media respectively. In addition, the buckled phase exhibits a lower recovery rate in visible light and ultraviolet regions for biomarkers than the puckered phase phosphorene. Conclusively, the buckled phosphorene tends to show remarkable sensitivity and a lower recovery rate than puckered phosphorene toward sensing COVID-19 biomarkers.

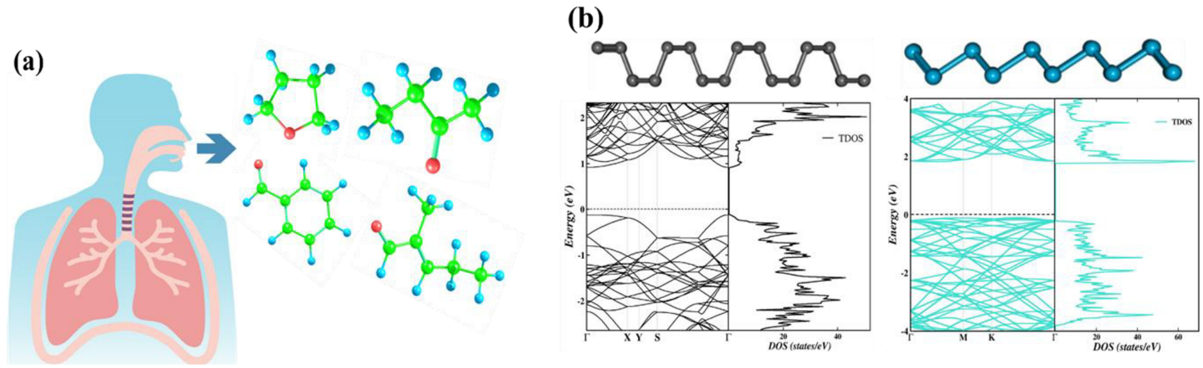

Figure 1. (a) Covid-19 biomarkers exhaled from infected lung, (b). Optimized Structures and Band/DOS plots of Black and Blue Phosphorene for sensing Biomarkers

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J-135

Interplay of Molecular Crowder Size, Hydrophobicity and Solvation in Determining Stability of Dimers and Tetramers

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The study of early stages of aggregated peptides within crowded environment [1] is of fundamental importance to understand the complex molecular mechanism of fibril formation, which are associated with neurodegenerative diseases like Alzheimer, Parkinson etc [2]. Recently, it was postulated that, along with the chemical nature of crowders present, associated water dynamics also play an important role in peptide aggregation and fibril formation [3,4,5,6]. In this study, we investigated the influence of increase in steric effect [7] and hydrophobicity [8] of molecular crowders along with the role of hydration water using Aβ(16-22) (that is known to be prone to aggregation to form amyloid fibrils [9]) dimer and tetrameric system in varying packing fractions. The crowders employed in this study are ethylene glycol (EG), diethylene glycol (DEG), and a modified diethylene glycol, where one hydrogen atom is replaced with a methyl group to make it more hydrophobic (UCON), in aqueous solution at both low and high packing fractions.

Smaller crowders, like ethylene glycol (EG), enhance the stability and compactness of β-sheet structures, while larger size crowders, such as diethylene glycol (DEG), destabilize these structures, particularly at higher packing fractions. With increasing the hydrophobicity and steric effect of crowders, more hydrophobic crowder (UCON) at low packing fraction maintain more compactness, and β-sheet content of protofibrils.

At low packing fractions, crowders disrupt the average tetrahedral order of water molecules and are preferentially adsorbed on protein surfaces, especially in tetramers, promoting the stability and compactness of the protofibril by promoting local crowding effects. At high packing fractions, this disruption is more pronounced, particularly with EG, the preferential binding coefficients become negative, indicating less interaction between crowders and proteins due to increased steric hindrance which destabilizes the oligomers. The diffusivity of water shows an anomalous behavior, implying that water molecules are confined due to the presence of crowders, at higher crowder concentrations. These results provide more insights into the complex interplay between chemical nature of crowder and hydration water dynamics in the formation of amyloid aggregates.

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J-136

Theoretical Investigation of the Surface Binding Sites in PET Hydrolases for Selective PET Binding

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Plastic biodegradation represents a promising strategy for upcycling plastic and managing plastic waste [1]. PET hydrolases, a group of enzymes within the α/β hydrolase family are known for their ability to hydrolyze PET [1]. To scale this process industrially, structure-based rational engineering is essential. Enzyme-substrate complex formation is a critical step in catalysis, as it determines the specificity of the reaction [2]. There are reports on mutations on PETases that enhance enzymatic activity.[3] But enzyme-substrate complex formation step has not been extensively studied. In this work, we attempt to explore the specificity of enzyme-substrate complexes in some wild-type and mutated PET hydrolases with the help of molecular dynamics simulations. Our findings revealed additional binding sites, and mutations at targeted sites have provided ways to improve the selective PET binding to the active site (Figure 1).

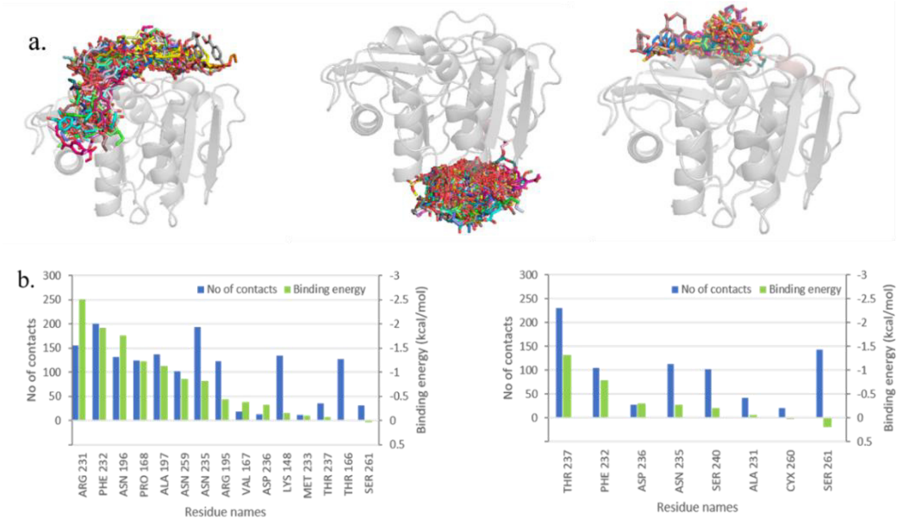

Figure 1: a. Three major clusters of tetrameric PET on surface of *Is*PETase b. Binding energy and contact plot of WT(left) and R231A mutant(right).

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J-137

Identification of HLA-DR Associated Peptides Involved in Beryllium Hypersensitivity

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Beryllium exposure leads to beryllium sensitization and Chronic beryllium disease (CBD) which is a granulomatous lung disease caused by accumulation of Be-responsive CD4$^+$ T-cells in the lower respiratory tract.[1] Beryllium hypersensitivity and CBD is mainly associated with HLA-DP alleles having glutamate residue at 69th position of β chain.[2,3] In HLA-DPGlu69 negative individuals, HLA-DRPhe47 is the susceptible marker of beryllium hypersensitivity.[4] However, the potential Be^{2+} binding site on the HLA-DR allele is unknown because the natural presenting peptide is unknown. Hence, molecular dynamics (MD) simulations were carried out to identify the appropriate peptide-Be^{2+} ion combinations that can bind to HLA-DR protein and to explore the potential binding site of Be^{2+} ion on the protein-peptide complexes [Figure 1a]. The Be^{2+} ion binds with HLA-DR protein and peptide simultaneously. Further, the peptide has a significant role in maintaining the structural stability of the Be^{2+}-HLA-DR system. The binding free energies between HLA-DR protein and peptides without and with Be^{2+} ion were evaluated to understand the most suitable peptide that could bind with Be^{2+} and HLA-DR protein [Figure 1b].

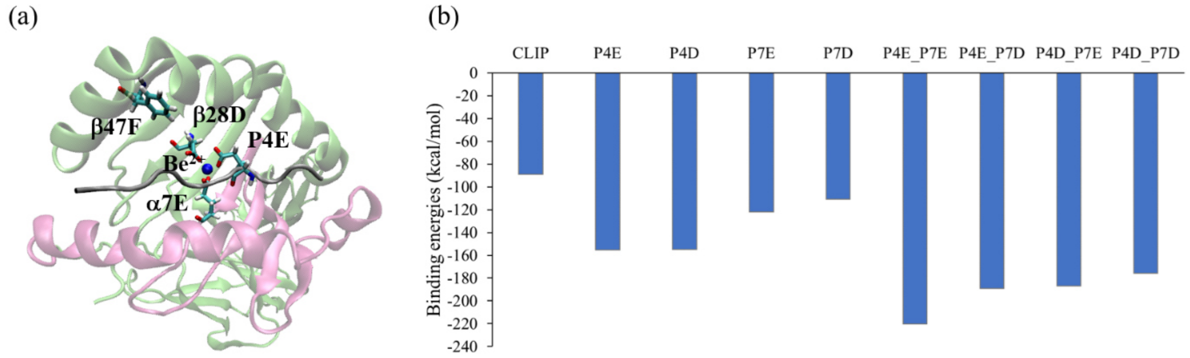

Figure 1. (a) Representative snapshot from MD simulation of the HLA-DR3_peptide_Be^{2+} complex. (b) Binding energies between protein and peptides without and with Be^{2+} ion

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J-138

Understanding the Mechanism Ice Nucleation and Ice Growth Inhibition Phenomena by Ice Binding Proteins (IBPs)

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The molecular mechanism behind the biological functions of ice binding proteins (IBPs) is yet to be understood completely. Also, what physical parameters differentiate between the IBP and non-IBP is largely unknown. IBPs can be categories into two groups: Ice nucleating proteins (INPs) and Antifreeze proteins (AFPs). INP promotes the process of ice nucleation whereas AFP assists to inhibit process of ice growth. To get an atomistic overview of nucleation and antifreeze activity of different classes of IBPs, we have studied ice growth from different ice surfaces in the presence of hyperactive Spruce budworm (sbw) AFP. Results are compared with the topologically similar non-AFPs. Simulation data suggest that the ice surface coverage is a critical factor in ice growth inhibition. Due to the presence of an ice binding surface (IBS), AFPs form a high affinity complex with ice, accompanied by a transition of hydration water around the IBS from clathrate-like to icelike. Several residues around the periphery of the IBS anchor the AFP to the curved ice surface mediated by multiple strong hydrogen bonds, stabilizing the complex immensely. In high surface coverage regime, the slow unbinding kinetics dominates over the ice growth kinetics and thus facilitates the ice-growth inhibition. Due to the non-availability of a proper ice binding surface, non-AFPs form low affinity complex with the growing ice surface. As a result, the non-AFPs are continuously repelled by the surface. If the concentration of AFPs is low, then the effective surface coverage is reduced significantly. In this low surface coverage regime, AFPs can also behave like impurities and are engulfed by the growing ice front. We have also explored the pre-binding scenario that how AFP recognize growing ice surface. AFP possesses strong affinity towards growing ice surface which leads to the synergy effect to the ice growth. We have found that antifreeze proteins can sense ice surface from certain distance apart and binds to the surface more quickly compare to the other class of proteins.

Structure of INP and AFP are more or less similar in terms of ordering and still higher than that of non-IBP i.e., INP have greater tendency to organize water molecules into ice like pattern compared to non-IBP which may be responsible for their potent ice nucleation activity. Ordering also increases with increased surface area for the INP, indicates that continuity of water organizing unit also critical for optimal activity. When we enhance the nucleation process using external force, it is found that water ordering near binding surface of INP is far better compared to the non-IBP. The overall picture is that predefined binding surface with optimal number of water- organizing motif enhance water ordering which in turn develops non-equilibrium like situation to the water molecules near binding surface of INP and by fluctuation ice cluster is formed.

J-139

Registry Alteration in Dynein's Microtubule-Binding Domain: A AAA domain-guided event

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Dynein is a motor protein essential for the cell due to its retrograde motion towards the nucleus. This study investigates the interaction between dynein's microtubule-binding domain (MTBD) and microtubules, emphasizing the role of the coiled-coil stalk in regulating binding states. Dynein, a motor protein, uses ATP hydrolysis to generate mechanical movement along microtubules [1], with the MTBD playing a critical role in binding and releasing from microtubules. Previous research suggested that the coiled-coil stalk primarily governs this interaction [2]. However, recent arguments propose a two-way communication mechanism where binding and unbinding may also influence dynein's nucleotide state [3].

Using all-atom explicit solvent simulations, enhanced sampling techniques, and coarse-grained methodologies, the study explores the effects of the stalk and microtubules on the structural stability of different MTBD conformations. We have found that the MTBD without the stalk and microtubule predominantly stays in a weak binding state. When a limited length of the stalk and microtubule interaction is introduced, a balance between strong and weak binding states is restored. The addition of a full-length stalk further stabilizes these states. The study also shows that in the presence of microtubules, the stalk's conformational change precedes the MTBD's, indicating that the AAA+ ring's nucleotide state influences the MTBD through the stalk. This produces a hysteresis in the MTBD cycle.

The findings suggest that the stalk is a guiding factor in MTBD state transitions, with the AAA domain modulating the stalk's registry. This study highlights the intricate mechanisms by which dynein's interaction with microtubules is regulated, emphasizing the stalk's crucial role in facilitating these binding state transitions.

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CTTC – 2024

Highlights of Activities of Various DAE Units

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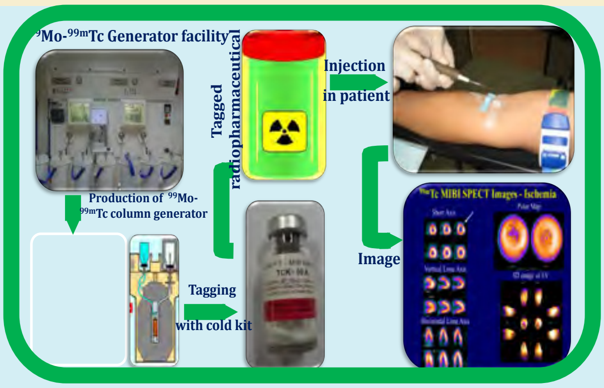

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प्रौद्योगिकीय संपदा के माध्यम से राष्ट्र का गौरवान्वयन
Creating Pride for the Nation through Technological Wealth

नाभिकीय एवं विशेष ग्रेड का भारी पानी
Nuclear & Special Grade Heavy Water

पोटैशियम धातु Potassium Metal

ड्यूटेरियम गैस Deuterium Gas

एनएमआर विलायक NMR Solvents
($CDCl_3$; Acetone-d6; DMSO-d6; Acetonitrile-d3 etc.)

बोरॉन-10&11 Boron-10&11

नाभिकीय ग्रेड सोडियम
Nuclear Grade Sodium

निष्कर्षण धातुकर्म हेतु विलायक
Solvents for Extractive Metallurgy

Supporting Fast Breeder Reactor Programme

Heavy Water & Allied Products

Nuclear Solvents

Technological Initiatives

Environment Care

Societal Initiatives

बहुविध गतिविधियां
Multifold Activities

स्वास्थ्य सेवा हेतु सामग्री
Materials for Healthcare
(पीईटी स्कॅनिंग हेतु ऑक्सीजन-18 जल
^{18}O Water for PET Scanning;
कैंसर के उपचार हेतु ड्यूटेरियम क्षीण जल
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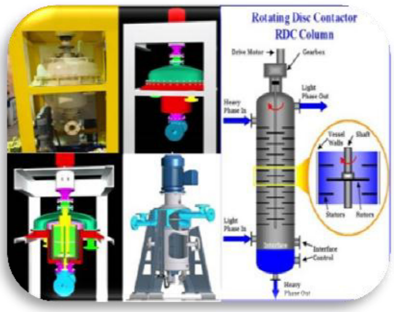

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Cloud covered hill @ Anushaktinagar

Blooming of Moss Rose @ Anushaktinagar