https://www.cttcmumbai.org.in

cttcmumbai@gmail.com



The DAE-BRNS Symposium Current Trends in Theoretical Chemistry (CTTC-2024) is being organized by Theoretical Chemistry Section, Chemistry Division, Bhabha Atomic Research Centre from 26 to 28 September, 2024. Formulation of newer and more powerful theoretical tools, cutting edge modelling strategies and robust simulation techniques form an ongoing and integral part of research activities in theoretical chemistry. In view of the nature and wide applicability of this subject, one of the major national needs is to bring various Indian researchers in a single platform to discuss current progress, challenges and pitfalls. 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 proceeding of the symposium will constitute keynote addresses, invited talks and presentation of contributory papers as posters.

Topics to be covered

- 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
- Computational Chemistry of Molecules and Materials under Extreme Conditions
- **Experiment Driven Theoretical Investigations**
- Modeling, Theory and Simulation for the Exploration of Biological Phenomena and Drug Design

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For further details, please contact

Convener, CTTC-2024

Theoretical Chemistry Section,

Chemistry Division,

Bhabha Atomic Research Centre, Trombay,

Mumbai 400085, INDIA

Fax: 91-22-2550 5331/5150/5151 Tel: 91-22-

2559 5607

Email: cttcmumbai@gmail.com



Organized by

Chemistry Division
Bhabha Atomic Research Centre
Mumbai – 400085, INDIA

In Association with

Society for Materials Chemistry
Chemistry Division
Bhabha Atomic Research Centre
Mumbai – 400085, INDIA

