



**DAE-BRNS National Workshop on**  
**“Atomistic Modeling of Molecules and Materials (AMMM-2023)”**  
**December 11-14, 2023**

**Venue:**  
**Multipurpose Hall, TSH**  
**Anushaktinagar, Mumbai-**  
**400094**



**Organized By:**  
**Chemical Engineering Group**  
**Bhabha Atomic research Centre**  
**Trombay, Mumbai – 400085**

**Atomistic Modeling of Molecules and Materials**

**AMMM-2023**

$F=ma$   $F=ma$   $F=ma$   $F=ma$   $F=ma$   $F=ma$

$H\psi=E\psi$   $H\psi=E\psi$   $H\psi=E\psi$   $H\psi=E\psi$   $H\psi=E\psi$   $H\psi=E\psi$

Machine Learning Laboratory

$g(r)$

$r(A^\circ)$

OW-OW  
OW-HW  
HW-HW

For further information, please visit at [http://www.barc.gov.in/symposium/ammm\\_2023](http://www.barc.gov.in/symposium/ammm_2023)

## **AIM & OBJECTIVES:**

A national workshop on “Atomistic Modeling of Molecules and Materials (AMMM-2023)” is being organized by Chemical Engineering Group, Bhabha Atomic Research Centre (BARC), Trombay, Mumbai, India, during 11<sup>th</sup>-14<sup>th</sup> December, 2023 at Multipurpose Hall, TSH, Anushaktinagar, Mumbai. The workshop is supported by the Board of Research in Nuclear Sciences (BRNS) and Department of Atomic Energy (DAE). Atomistic modeling has significantly contributed to the establishment of computer simulations as the third pillar of science, together with experiments and theory. Atomistic modeling techniques incorporate atomic-level information to simulate macroscopic properties of materials through its molecular building blocks. It involves many disparate fields of science, ranging from classical and statistical mechanics to quantum chemistry, numerical methods, or algorithmic developments. The growing power of parallel computations has spurred the development of methods and code interfaces, widening the potential of simulations to tackle a wide range of scientific issues and placing tools in the hands of a wider group of scientists. The computational techniques of atomistic simulation coupled with machine learning (ML) and artificial intelligence (AI) offer an avenue to rapidly invent new materials and navigate this enormous space to infer complex design principles and identify high-quality candidates more rapidly than trial-and-error experimentation. The workshop is proposed to bring together the experts in first principles electronic structure calculations and molecular dynamics centered atomistic modeling and ML/AI based molecular simulations from DAE and other research institutes for imparting training to the young students, scientists and faculties at the starting of their scientific carrier. The workshop will cover the following topics.

## **SCOPE OF WORKSHOP:**

- 1. Computational Modeling of Lanthanides-Actinides and Isotope Separation**
- 2. Atomistic Modeling of Multi-Component Glasses**
- 3. Atomic and Electronic Structure Understanding of Radiation Damage to Materials**
- 4. Theory and Computation on Molecular Transport Phenomena and Spectroscopy**
- 5. Computational Thermodynamics of Nuclear Materials**
- 6. Atomistic Modeling of Catalyst and Design of Hydrogen Storage Materials**
- 7. Atomistic Understanding of Rechargeable Batteries**
- 8. Machine Learning and Parallel Computing Accelerated Atomistic Modeling**

## **PATRON**

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## Abstract Submission

Contributory papers are invited on topics listed in the scope in the form of one page manuscript in specified format. The entire text should be typed in MS Word, paper size A4(210 x 297 mm), page margins: top 25 mm, bottom 25 mm, left 25 mm and right 25 mm. The font should be Times New Roman (font 12) with single line spacing. Manuscript should be categorized (1 to 8) as per the titles given under **SCOPE OF WORKSHOP**.

E-mail ID of corresponding author should be given in the manuscript and presenting author should be underlined. All the future communications in respect of manuscript will only be made to corresponding author. DAE participants may please note that the contributed papers should be accompanied with scanned copy of the note of approval from the competent authority. Accepted abstract without registration will not be considered. Short-listed abstract will be selected for flash presentation.

### Registration fee

Research student/Postdocs	Rs. 2000
Faculty/Scientist	Rs. 4000
Participants from industry	Rs. 8000

### Important Dates

Abstract submission opening	15-10-2023
Final abstract submission	30-10-2023
Acceptance notification	10-11-2023
Registration/Accommodation (Start)	10-11-2023
Registration/Accommodation (Last)	20-11-2023

**Registration fees will be accepted only through crossed cheque/crossed DD/Net banking system to the following account**  
**Beneficiary name : Society for Atomistic and Continuum Modeling**

**Name of the Bank : State Bank of India**  
**Branch code : 01268**  
**Account number : 41974598642**  
**IFSC code (INDIA) : SBIN0001268**

**Note:** The manuscript must be submitted via e-mail only at [ammm2023barc@gmail.com](mailto:ammm2023barc@gmail.com)

## ACCOMMODATION

Hostel accommodations on double sharing basis will be provided to students. Other participants can book single/twin-sharing AC rooms in our guest house. Accommodation requests should be made through email only at **ammm2023barc@gmail.com**. Please note that accommodation in hostels and guest house is limited and would be provided only after receipt of an advance payment on first come first service basis. Those who want to book accommodation in nearby hotels can directly book the accommodation by contacting hotels.

Twin sharing non-AC hostel room for students (per person): Rs. 1000/- (for full symposium)

Twin sharing AC double bedded room in our guest house (per person per day): Rs. 1000/-

VIP suit in our guest house (per person per day): Rs. 3000/-

## BOARD OF RESEARCH IN NUCLEAR SCIENCES (BRNS)

Board of Research in Nuclear Sciences (BRNS) supports research and development activity in universities, institutes of higher learning and national laboratories in India in the fields relevant to the mandate of Department of Atomic Energy. BRNS also supports symposia, conferences, seminars and workshops in various areas of science and technology.

## ABOUT THE VENUE

Mumbai is India's most cosmopolitan city, finance and business capital and home to the entertainment industry. Mumbai is a vibrant, pulsating metropolis, which affords diverse sightseeing opportunities. There are unlimited tourist attractions in and around Mumbai for visitors of all ages and culture. These places can refresh the spirits and provide a perfect retreat to visitors, like the beautiful and fun filled beaches of Juhu, Elephanta caves, Marine drive, Hanging garden, breathtaking scene of hill stations like Matheran and Lonavala, pilgrimage and spiritual centers suiting every faith, star studded Bollywood, Old pubs and vineyards.....a bit for everyone.



## How to reach BARC

The Bhabha Atomic Research Centre (BARC) is located near Anushakti Nagar Bus Terminus, Mumbai. Anushakti Nagar Bus Terminus is a landmark known to most taxi/auto drivers. More details are available on <http://barc.gov.in/visitor/index.html>



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