

DAE-BRNS

Symposium on Advances in Atomistic and Continuum Modeling  
(DAE-SAACM2024) during 23-26 October, 2024



DAE Convention Centre,  
Anushaktinagar  
Mumbai 4000 94

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



## AIM & OBJECTIVES

A four day national symposium on “DAE Symposium on Advances in Atomistic and Continuum Modeling (DAE-SAACM2024)” is being organized by Chemical Engineering Group, Bhabha Atomic Research Centre (BARC), Trombay, Mumbai, India, during 23-26 October, 2024 at DAE Convention Centre, Anushaktinagar. The symposium is held in association with Society for Atomistic and Continuum Modeling (SACM) and supported by the Board of Research in Nuclear Sciences (BRNS), Department of Atomic Energy (DAE). Atomistic modeling comprising of electronic structure calculations and molecular dynamics simulations is decisively used to estimate the properties and behavior of molecules and materials-even before their creation. Additionally, machine learning (ML) and artificial intelligence (AI) have accelerated the molecular search space which has boosted the design & development of complex chemical system. Atomistic simulations often require high computational resources due to the large number of atoms involved and the complexity of the inter-atomic interactions. Conversely, continuum modeling may comprise large spatial domains and long time scales, further adding to the computational burden. Integrating atomistic and continuum models while maintaining computational efficiency remains a formidable task. The behavior of materials at the atomic scale can significantly influence macroscopic properties, but bridging these scales requires robust methodologies for transferring information between atoms to continuum. Developing effective coupling algorithms that preserve the accuracy and consistency of data across scales is essential for reliable multiscale simulations. Further, Quantum computing has the potential to revolutionize the field of science & technology by accelerating the multiscale modeling with enormous computational capabilities that surpass classical computers. The symposium is proposed to bring together the experts in Electronic Structures and Atomistic Simulations, Continuum Modeling, ML, AI, Parallel and Quantum computing from DAE and other research institutes for exchange of ideas among research scholars, scientists and faculties. The symposium will cover the following topics.

## SCOPE OF THE SYMPOSIUM

1. Computational Modeling of Lanthanides-Actinides and Isotope Separation
2. Atomistic Modeling of Multi-Component Glass
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 Battery
8. Atomistic Simulations of Biological Systems
9. Machine Learning and Artificial Intelligence Accelerated Atomistic Modeling
10. Parallel Computing and Quantum Computing Accelerated Atomistic Modeling
11. CFD and Mathematical Modelling for Applications in Nuclear Fuel Cycle
12. Applications of CFD and Mathematical Modelling in Thermal Hydraulics
13. CFD and Mathematical Modelling for Applications in Chemical Engineering
14. CFD and Mathematical Modelling for Applications in Nuclear and Chemical Process Safety
15. Emerging Materials
16. Advanced Characterization and Processing Techniques



## PATRON

A.K. Mohanty - Chairman, Atomic Energy Commission (AEC)

Vivek Bhasin - Director, Bhabha Atomic Research Centre (BARC)

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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 16) as per the titles given under SCOPE of the symposium.

The manuscript should be submitted online via website : [www.sacm.org.in/DAE-SAACM-2024](http://www.sacm.org.in/DAE-SAACM-2024)  
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. Some abstracts will be selected for oral presentation.

## AWARDS

There will be award for best oral and poster presentation. Also "Atomistic Modeler and Continuum Modeler of the year 2024" medal will be conferred by SACM to the best researcher who has received their PhD after 15th August, 2021. The eligible candidate is requested to submit CV, list of publications and an abstract (300 words) of application of their research findings to the convener of DAE-SAACM2024 on or before 15th September, 2024. For details please visit: [www.sacm.org.in](http://www.sacm.org.in)

### Registration fee

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

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

### Important Dates

Abstract submission opening	: 17-07-2024
Last date of abstract submission	: 31-08-2024
Last date of acceptance	: 10-09-2024
Registration/Accommodation	: 15-09-2024

## 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 at website (<http://www.sacm.org.in>) email:saacm2024barc@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.

Type of accommodation	Amount	Period
Twin sharing non-AC hostel room for students (per person)	Rs. 1000	Full symposium
Twin sharing AC double bedded room in our guest house(per person)	Rs. 1000	Per day
VIP room guest house (per person)	Rs. 3000	Per day

## 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, Filmcity, 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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For updates please visit our website :

[www.sacm.org.in/DAE-SAACM-2024](http://www.sacm.org.in/DAE-SAACM-2024)

