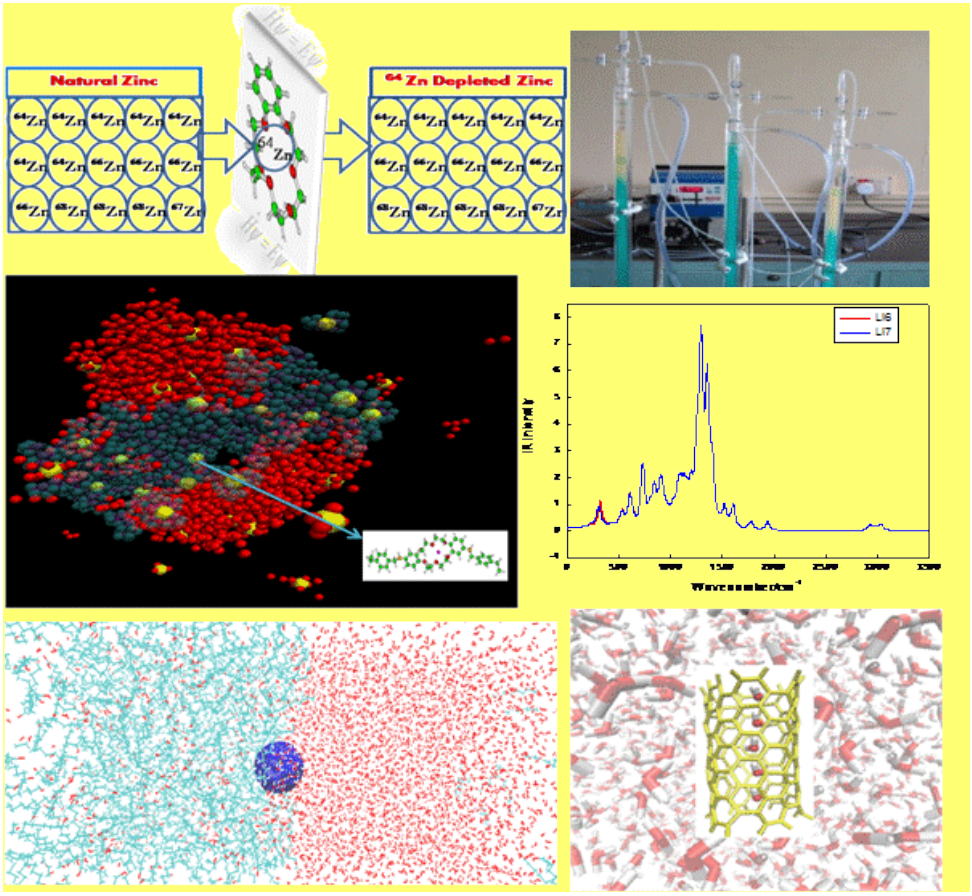
DAE- BRNS sponsored Theme Meeting on

Application of Molecular Modeling in Separation Processes

AMMSP2015

On

January 16, 2015



Venue:
C Block Auditorium, Mod Lab
Bhabha Atomic Research Centre

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

Scope of the theme meeting:

One day theme meeting on "***Applications of Molecular Modeling in Separation Processes***" is being organized by Chemical Engineering Division, Bhabha Atomic Research Centre (BARC), Trombay, Mumbai, India, on January 16, 2015. The meeting is supported by the Board of Research in Nuclear Sciences (BRNS), Department of Atomic Energy (DAE).

The power of molecular modeling is growing rapidly with the continuing development of computer power, new and robust algorithms, and the availability of software. Today molecular modeling can sometimes provide useful estimates of the properties and behavior of materials- even before they have been synthesized and useful estimates of the parameters and behavior needed to do traditional chemical engineering process development & design. The theme of the meeting is contemporary research on molecular modeling for the development and design of chemical engineering systems and processes. The deliberations of the theme meeting will cover the **molecular modeling aided studies** on following topics:

1. **Isotope separation**
2. **Nuclear waste reprocessing and purification**
3. **Desalination and water**
4. **Adsorptive separation on catalytic surfaces**
5. **Fundamental studies on structures, thermodynamics and transport properties**
6. **Nanoparticles and polymers**

Patron

S. Basu, Director, BARC

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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.

ADDRESSES FOR CORRESPONDENCE

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Those who are willing to participate please contact secretary, organizing committee through e-mail (Consent of Head of the Division is necessary).

Last date of registration: January 5, 2015

DAE-BRNS Theme Meeting on Application of Molecular Modeling in Separation Processes

(AMMSP2015)

January 16, 2015

Venue: C Block Auditorium

Bhabha Atomic Research Centre

Scientific programme

Registration	8.30-10.00
Inauguration	10.00-10.30
Tea	10.30-11.00

Session-I (11.00-1.00) (Chair: P.K. Wattal)

1. Molecular Simulation of Diffusion and Selective Complexation in Separation Processes
   Prof. V.G. Gaikar, ICT, Mumbai (11.00-11.30)
2. Theoretical Prediction and Experimental Validation of New Actinide Selective Ligands
   Dr. T.K. Ghanty, BARC, Mumbai (11.30-12.00)
3. Molecular Modeling Guided Experiments for Separation of Isotopes and Metal Ions
   Dr. Sk. M. Ali, BARC, Mumbai (12.00-12.30)
4. Molecular Simulations in a Computational Scheme for Rational Solvent Design: Extraction of R-PAC
   Prof. J. Adhikari, IIT, Mumbai (12.30-1.00)

Lunch break: 1.00-1.45pm (Mod Lab canteen)

Session-II (1.45-4.00pm) (Chair: P.K. Tiwari)

5. A Computational Perspective on Non-Covalent Interactions and its Relevance to Separation Science
   Dr. G.N. Sastry, IICT, Hyderabad (1.45-2.15)
6. Coarse-grained Molecular Simulations of Polymers and Nanocomposites
   Prof. J. Singh, IIT, Kanpur (2.15-2.45)
7. Fluids in Nanochannels and Nanopores: An Envisaged through Molecular Dynamics Simulations
   Dr. N. Choudhury, BARC, Mumbai (2.45-3.15)
8. A First Principles Approach to Materials Modeling: Implications toward H - Economy
   Dr C. Majumdar, BARC, Mumbai (3.15-3.45)

Tea Break 3.45-3.55

Session-III (3.55-5.30pm) (Chair: B.N. Jagatap)

9. Unusual Dynamical Features of Hydrocarbons Adsorbed in Porous Media: MD Simulation Study
   Dr. S. Mitra, BARC, Mumbai (3.55-4.25)
10. Dynamical Correlations and Negative Maxwell Stefan Diffusivities for Molten Salt LiCl-KCl and LiF-BeF2
    Dr. B. Chakraborty, BARC, Mumbai (4.25-4.55)
11. DFT Modeling on Functionalized Carbon Nanomaterials for Adsorptive Separation of Metal ions
    A.K. Singha Deb, BARC, Mumbai (4.55-5.15)

Concluding remarks 5.15