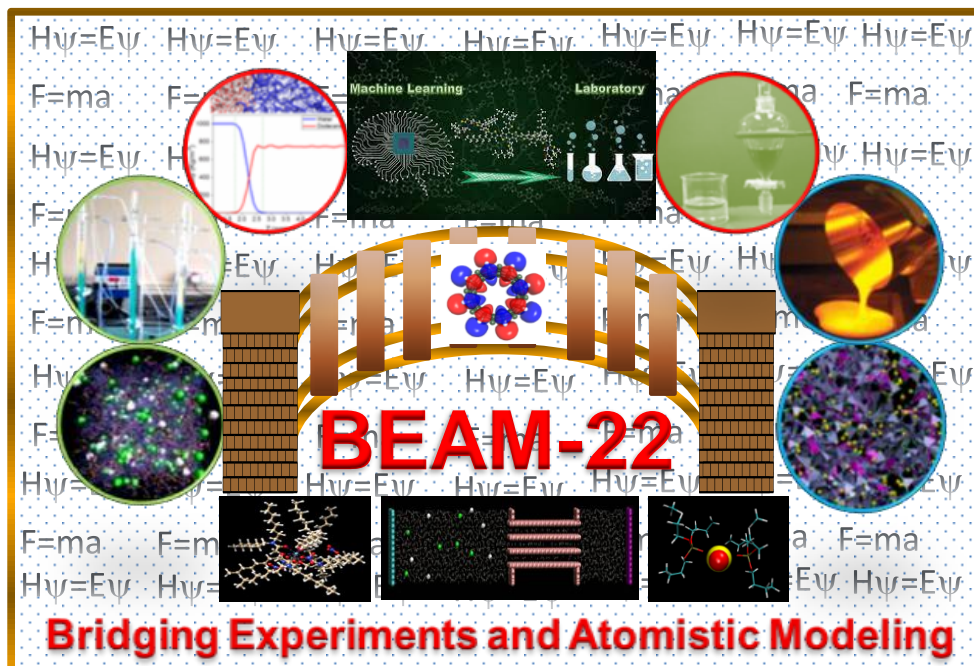




Proceedings of
DAE- BRNS Theme Meeting

“Bridging Experiments and Atomistic Modeling (BEAM-22)”

Friday, November 4, 2022



Venue:

Multipurpose Hall, TSH
Anushaktinagar, Mumbai

Organized By:

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

DAE- BRNS Theme Meeting

“Bridging Experiments and Atomistic Modeling (BEAM-22)”

Friday, November 4, 2022

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Scientific Programme

Registration 8.30-10.15

Inauguration 9.15-9.30

High Tea 9.30-10.15

Session-I (10:15-11:55) (Chair: Prof. Tamal Banerjee)

Plenary Lecture

1. PAMAM dendrimer in Supercapacitor and uranyl filtration applications
Prof. Prabal K. Maiti, IISc, Bangalore (10:15-10:45)

Invited Lecture

2. Materials for alternative energy synergy between atomistic modeling and experiments
Prof. Prasenjit Sen, HRI, Prayagraj (10:45-11:10)
3. Counter-intuitive adsorption behavior of ions on charged surface
Prof. Ateeque Malani, IIT, Mumbai (11:10-11:35)
4. New Outlook into the Noble Gas Chemistry
Dr. T.K. Ghanty, BARC, Mumbai (11:35-12:00)

Session-II (12:00-13:15) (Chair: Prof. Ateeque Malani)

5. Modern Machine Learning methods for molecular design
Prof. U. Deva Priyakumar, IIIT, Hyderabad (12:00-12:25)
6. Evolution equations for the short-range order parameter: Application to problems in catalysis, adsorption and alloy materials
Prof. Abhijit Chatterjee, IIT, Mumbai (12:25-12:50)
7. Computational design of novel Deep Eutectic Solvent with desired properties
Prof. D.K. Maity, HBNI, Mumbai (12:50-13:15)

Lunch break: 1.15-14.15 pm

Session-III (14:15-15:55) (Chair: Prof. Prasenjit Sen)

8. Buckling and Defects in Two - Dimensional Atomically Thin Monolayers
Prof. Ayan Datta, IACS, Kolkata (14:15-14:40)
9. Atomistic design of adsorbents: Computer to chromatographic column
Dr. SK. Musharaf Ali, BARC, Mumbai (14:40-15:05)
10. Thermodynamical Properties of Nuclear Materials
Dr. Ashok Arya, BARC, Mumbai (15:05-15:30)
11. Quantum chemical and molecular dynamics insights for the extraction of pharmaceutical moieties from aqueous environment Using menthol-based hydrophobic eutectic solvents
Prof. Tamal Banerjee, BARC, Mumbai (15:30-15:55)

Tea break: 15:55-16:15

Session-IV (16:15-17:40) (Chair: Dr. Anil Boda)

12. Stabilization of vaccinal RNA in D₂O and eliminating the cold chain
Dr. Tusar Bandyopadhyay, BARC, Mumbai (16:15-16:40)
13. How Osmolytes balance surface charges under Salt-stress
Prof. Jagannath Mandal, TIFR, Hyderabad (16:40-17:00)
14. Predicting microstructures of polymer blends and composites using AI and molecular simulations
Prof. Tarak Patra, IIT, Chennai (17:00-17:20)
15. Atomistic Design and decoding of multicomponent glass
Dr. Pooja Sahu, BARC, Mumbai (17:20-17:40)

Concluding Session-V (17:40-18:40) (Chair: Shri K.T. Shenoy)

Panel discussions

Forwarded

We welcome you all to the theme meeting organized by Chemical Engineering Division, ChEG, Bhabha Atomic Research Centre, Trombay, Mumbai, India. The theme meeting is supported by the Board of Research in Nuclear Sciences (BRNS), Department of Atomic Energy (DAE) and is being held in multipurpose hall, TSH, Anushaktinagar. Since the arrival of electronic computers in the past century, numerical methods for computing static and dynamic properties as well as thermo-physical parameters of chemicals have revolutionized atomistic modeling and have resulted in evolution of numerous software and hardware technology. Atomistic modeling aims at understanding and designing of novel molecules and materials in the field of chemistry, material science, physics, chemical engineering, separation science, medical science and bioscience. It provides valuable information, particularly in situations in which experiments are not feasible due to extreme conditions or some other practical constraints. Many notable scientists from the field of atomistic modeling will share their expertise with the participants in BEAM-22. We sincerely thank all of them for their consent and timely submission of abstracts.

We are extremely grateful to all the members of Advisory committee for their valuable guidance and support in formulating and shaping the theme meeting. The guidance, support and encouragement received from Shri K.T. Shenoy, Director, Chemical Engineering Group and Chairman, Organizing Committee during the entire process has been really gratifying and is being sincerely acknowledged. We are also grateful to Dr. S. Mukhopadhyay, Head, Chemical Engineering Division for her suggestions and support in each step of the theme meeting.

About 100 delegates from DAE and non-DAE institutes are participating in this theme meeting. Total 15 invited lectures were received. This theme meeting will provide a platform for having close and fruitful interaction among various experimental and theoretical research groups of DAE and other premier institutes of the country. This is expected to generate new ideas and will give the young researchers an opportunity to formulate their research in the frontier area of atomistic modeling based science and technology.

For hosting this event, the Organizing Committee received help, support and encouragement from different quarters and we acknowledge all of them. We sincerely thank NR&ChEG Board and Trombay Council for giving consent to organize the BEAM-22. We are grateful to all the organizing committee members for their efforts. We acknowledge the sustained support and cooperation extended by scientific/technical/non-technical staff of Chemical Engineering Group in organizing the theme meeting. We thank all the invited speakers, session chairpersons, faculty members, research scholars and students for their participations in this meeting. The Organizing Committee is grateful to Board of Research in Nuclear Sciences (BRNS) for financial assistance.

*Convener
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डॉ. अजित कुमार मोहान्ती
Dr. Ajit Kumar Mohanty

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सदस्य, परमाणु ऊर्जा आयोग
Member, Atomic Energy Commission



MESSAGE

I am delighted to know that a one day Theme Meeting on “Bridging Experiments and Atomistic Modelling” (BEAM) is being organized by Chemical Engineering Division, BARC, Mumbai on 4th November, 2022 at MPH, Training School Hostel, Anushaktinagar.

Scientists are utilizing Computer simulations as a direct route to explore the macroscopic observations of molecular systems of experimental interest from microscopic view. Given the unmet scientific needs associated with agility of development and testing the new ideas and paradigms, computer simulations can provide useful estimates of the properties and behaviour of materials even before they have been synthesized and evaluated through experiments. Atomistic modelling aims at understanding and designing of novel molecules and materials in the field of chemistry, material science, physics, chemical engineering, separation science, medical science and bioscience. The speakers will cover the theme computation and innovation from different perspectives. I am privileged to say that this theme meeting will provide the home and focal point for bridging and interfacing different simulation communities to do a new level of science and great challenge problems, which will definitely offer suitable solutions to numerous global issues. These programmatic subjects should shed further light on microscopic and nanoscopic view of various fields that could potentially be leveraged and optimized for rapidly emerging ideas especially with the integration of machine learning or artificial intelligence.

I congratulate the organizers for planning this Theme Meeting which will benefit in further advancement of this thrust area of research some of which might help in the development of cutting edge technology. I am sure the present Theme Meeting will provide platform for having a close and fruitful interaction of various experimental and theoretical research groups of BARC and other premier institutes of the country. This is expected to generate new ideas and will give the young researchers an opportunity to formulate their research in the frontier area of atomistic modelling and its bridging with experiments.

I wish a grand success to BEAM-22 Theme Meeting.

Ajit Kumar Mohanty
(Dr. Ajit Kumar Mohanty)



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आज़ादी का अमृत महोत्सव

PAMAM dendrimer in Supercapacitor and Uranyl filtration applications

Prabal K Maiti
Department of Physics
Indian Institute of Science

Using fully atomistic molecular dynamics (MD) simulations, we investigate the performance of hyper-branched poly(amidoamine) (PAMAM) dendrimer as an electrolyte and an electrode coating material in a graphene-based supercapacitor. We investigate the performance of the capacitor using two different modeling approaches, namely the constant charge method (CCM) and the constant potential method (CPM). We found that the presence of the dendrimer in the electrodes and the electrolyte increased the capacitance by about 65.25% and 99.15% respectively, compared to the bare graphene electrode-based aqueous

EDLCs. We will also discuss a novel strategy to extract uranyl (UO_2^{2+}) ions from aqueous conditions with the help of PAMAM [poly(amido)amine] dendrimers. Using atomistic MD simulations, we explore the adsorption behaviour and properties of aqueous solutions of UO_2^{2+} ions in the vicinity of PAMAM dendrimer, with a focus on the interactions of the UO_2^{2+} ions with the PAMAM dendrimer, and their adsorption mechanism. We find that the adsorption of UO_2^{2+} ions in PAMAM dendrimer decreases significantly as the pH level of the aqueous solution increases. The mechanistic insights obtained in this work reveal that the PAMAM dendrimers can be reused as chelating agents.

References:

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2. Tarun Maity, Abhishek Aggarwal, Subhadeep Dasgupta, V Vasumathi, A. K. Singha Deb, Sk. M. Ali, and Prabal K Maiti, Atomistic molecular dynamics provide insights to efficient removal of UO_2^{2+} ions using poly (amidoamine) dendrimer, (to be submitted).

Materials for alternative energy

Synergy between atomistic modeling and experiments

Prasenjit Sen

Harish-Chandra Research Institute, Chhatnag Road, Jhansi, Prayagraj (Allahabad), UP.

Need for identifying alternatives to fossil fuel as sources of energy cannot be overstated. In our efforts to make a switch to alternative technologies, materials research has a big role to play, both in energy harvesting and storage. Synergy between our use of state of the art computational techniques and the experimental works of our collaborators have resulted in new insights and breakthroughs in these areas. In this talk I will touch upon three different works related to energy technologies. First I will present how we used high throughput computation to screen a class of ternary transition metal tri-chalcogenide materials to identify efficient hydrogen evolution reaction (HER) catalysts. These and further computational analyses identified ten new materials, of which, our experimental collaborators are attempting to synthesize a few. The second work will show how our first principles calculations based on density functional theory provided new insights into the mechanism of HER in alkaline media. Finally, I will present how our work on a candidate cathode material for rechargeable Zn-air batteries explains experimental observations, and may aid in practically achieving this technology.

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Counter-intuitive Adsorption Behaviour of Ions on Charged Surface

Sai Adapa and Ateeque Malani*

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Adsorption of ions at the solid - aqueous interface is the primary mechanism in fast biological processes to very slow geological transformations. Despite, little is known about role of ion charge, hydration energy and hydration structure on competitive adsorption of ions, their structure and coverage at the interface. In this report, we investigate the structure and adsorption behavior of monovalent (Rb^+ and Na^+) and divalent (Sr^{2+} and Mg^{2+}) cations ranging from 0-4.5 M of bulk concentrations on the muscovite mica surface. Divalent ions have stronger adsorption strength compared to monovalent ions due higher charge. However, we observed counter-intuitive behavior of lesser adsorption of divalent cations compared to monovalent cations. Our detailed analysis reveals that hydration structure of divalent cations hinders their adsorption. Both, Na and Rb ions exhibits similar adsorption behavior, however, the adsorption mechanism of Na^+ ions is different from Rb^+ ions in terms of redistribution of the water molecules in their hydration shell. In addition, we observed surface mediated RbCl salting out behavior, which is absent in Na^+ and divalent ions. We observed direct correlation in hydration energy of cations and their adsorption behavior.

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New Outlook into the Noble Gas Chemistry

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The noble gas elements were always considered to be inert prior to the discovery of XePtF₆ compound^[1]. After this discovery, numerous krypton and xenon containing oxide and fluoride compounds were synthesized. The discovery of first covalently bonded argon compound (HArF) has created immense interests among researchers to study various new ionic and neutral noble gas insertion compounds^[2]. Most of the reported noble gas insertion compounds are either neutral or cationic in nature while very few mono-anionic oxygenated or fluorinated noble gas inserted compounds are reported. The formation of a bond between noble gas element and electron rich anionic (nucleophilic) species is difficult because of the high negative electron affinity of noble gas elements and it requires a stronger electrophile to form a chemical bond. However, the [B₁₂Cl₁₁]⁻ and [B₁₂(CN)₁₁]⁻ species, in spite of being negatively charged, possess unprecedented counterintuitive super electrophilic behaviour and forms a covalent bond with the noble gases (B-Ng).^[3] Apart from fundamental understanding on the structure and bonding aspects of noble gas atom containing molecules, in recent years designing material for trapping of radioactive noble gases has attracted considerable interests.

Here, we will discuss the chemistry of various computationally predicted neutral, cationic noble gas compounds and mainly focus on the exceptional counter intuitive super electrophilic behaviour of [BeB₁₁(CN)₁₁]²⁻ dianion and its unusual covalent bonding with the noble gas elements.^[4] In addition, we will also discuss how the stability of unstable multi-charged anion in gas phase can be enhanced via insertion of a negative electron affinity Ng atoms. The insertion of a Ng atom in each B-F bond of B₁₂F₁₂²⁻ leads to formation of an unprecedented stable icosahedral B₁₂Ng₁₂F₁₂²⁻ dianionic compound where the second excess electron is very strongly bonded in the B₁₂Ng₁₂F₁₂²⁻ than in its parent B₁₂F₁₂²⁻ dianion.^[5]

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Modern Machine Learning Methods for Molecular Design

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Last few years witness a major surge in the use of modern machine learning methods in research in fundamental sciences. These methods have had phenomenal success in the technology areas such as computer vision, speech recognition, natural language processing (NLP), etc. This has inspired chemists and biologists to apply these algorithms to problems in natural sciences. Availability of high performance Graphics Processing Unit (GPU) accelerators, large datasets, new algorithms, and libraries has enabled this surge. ML algorithms have successfully been applied to various domains in molecular sciences by providing much faster and sometimes more accurate solutions compared to traditional methods like Quantum Mechanical (QM) calculations, Density Functional Theory (DFT) or Molecular Mechanics (MM) based methods, etc. Some of the areas where the potential of ML methods are shown to be effective are in drug design, prediction of high-level quantum mechanical energies, molecular design, molecular dynamics materials, and retrosynthesis of organic compounds, etc. In this presentation, we will take some examples of applied ML to chemical sciences, and discuss the importance of these methods in the context of existing computational tools.

Evolution equations for the short-range order parameter: Application to problems in catalysis, adsorption and alloy materials

Prof. Abhijit Chatterjee

Department of Chemical Engineering
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In multi component systems, such as the ones typically encountered in catalysis, alloy materials and energy materials, etc., the constituent atoms and molecules typically order/arrange themselves in a manner that is far from perfectly-random. The short-range order (SRO) parameter often becomes a useful mathematical quantity for the global structure in such cases. SRO refers to the likelihood of finding atoms/molecules of a particular type, in the vicinity of others atoms of same/another type. The SRO parameter is dictated by both micro- and macro-scopic parameters, such as interactions, thermodynamics and kinetics (reactions, diffusion, and other transport processes). I will discuss evolution equations for the SRO parameter. These equations can help provide an accurate picture of the thermodynamics and kinetic behavior in a variety of complex systems. Examples will be provided on how the formalism can bridge experiments and atomistic methods.

Computational design of novel Deep Eutectic Solvent with desired properties

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Computational study on a novel deep eutectic solvent (DES) consisting of choline acetate as the hydrogen bond acceptor (HBA) and malonic acid as the hydrogen bond donor (HBD) will be presented.¹ Electronic structure calculations have been performed on a series of HBAs and HBDs, out of which this particular pair with 1:2 eutectic composition found to be best suited to form redox and radiation stable DES. The eutectic composition is predicted from the computed phase diagram. Theoretical results suggest this DES to be more stable than the most popular DES, namely, reline. This is reflected from its huge lowering in melting point indicating formation of strong hydrogen bonds among the components. Experimental results on radiolytic yield of hydrogen shows this DES to be quite stable and comparable to the radiolytic stability of aromatic ionic liquids. The use of choline acetate as HBA in the new DES can open up varied possibilities of its applications starting from enzyme based industrial processes to separation science and technologies.

Reference

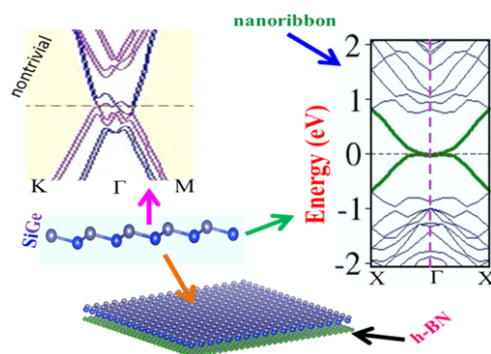
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Buckling and Defects in Two - Dimensional Atomically Thin Monolayers

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Graphene has emerged as one of the most fascinating areas of research in condensed matter and materials science. Apart from graphene, several other 2D analogues like silicene, phosphorene, MXenes, MoS₂, germanene have been recently isolated and characterized. One unifying theme among these new materials is that unlike graphene, they are non-planar. The mode and measure of the buckling (puckering) from planarity depends on the local electronic structure. The effects of such ripples are manifold particularly in its local reactivity to halogens and hydrogens along the more $\sim sp^3$ atoms. Pseudo Jahn-Teller (PJT) distortions is shown as a central unifying concept that explains the overall structural preferences of these systems. The extent of buckling also leads to interesting and emerging phenomenon like phase-transitions into Topological Insulators from normal semi-metal due to spin-orbital coupling (SOC). The effect of PJT in bestowing structural diversity and novel electronic and spin phases in 2D-monoatomic layers will be discussed in this lecture. How to utilize them for CO₂ conversion to useful chemicals will envisioned.



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Atomistic design of adsorbents: Computer to chromatographic column

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The use of solid adsorbent materials for the extraction of metal ions and isotope separation has many advantages over solvent extraction techniques because of generation of low volume of secondary waste, prevention of aqueous solubility loss of ligand, no requirement of large volume of flammable and volatile organic solvent and phase modifier. Therefore ligand functionalized adsorbents are emerging as a potential candidate for isotope separation of element and multi-component metal ions purification.

Macrocyclic crown ether is considered to be one of the wonder molecules due to its metal ion recognition ability. One such crown ether, 4',4'(5'')-di(tert-butylcyclohexano)-18-crown-6 (DtBuCH18C6) shows high selectivity toward Sr²⁺ ion in liquid-liquid extraction process. Crown ether cavity and Sr²⁺ ion size matching is one of the prime factor for selectivity. DtBuCH18C6 is prepared from dibenzo-18-crown-6 (DB18C6). Both have almost similar cavity and hence DB18C6 based resin should also show similar selectivity for Sr²⁺ ion. Owing to this, DB18C6 functionalized chloromethylated polystyrene (CMPS-DB18C6) resin was designed, synthesized and tested for Sr²⁺ ion uptake.

The metal ion recognition ability of macrocyclic crown ether can be used for isotopic recognition of element also. Macrocyclic adsorbent has been developed employing combined theoretical and experimental approaches. The prepared crown ether appended resin displays good adsorption capacity and isotope separation of gadolinium. The findings employing collective computational and experimental approaches might help in the design and improvement of future gadolinium isotopic enrichment processes using chemical exchange methods.

Crown ethers on functionalization with carbon nanotubes (CNTs) can be employed as a specific metal ion filter by exploiting its differential interaction with the metal ions. Therefore, by combining both computational and experimental studies, a new variety of nanoadsorbent has been developed.

Development of suitable adsorbents for the isotope separation and adsorptive purification of metal ions by means of experiment alone is somewhat time consuming and costly business. Molecular engineering, encompassing density functional theory, molecular dynamics simulations and statistical mechanics are reasonably well established for understanding the molecular level phenomena and thus is central for guiding the difficult experiments like isotope separation of element and multi-component metal ions purification. The present talk will discuss how the atomistic modeling can be exploited to construe the experimental results and plan future experiments.

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Thermodynamical Properties of Nuclear Materials

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Thoria (ThO_2) has the potential for use in nuclear energy applications with a high fuel performance as well as the additional advantages of less radiotoxic nuclear waste generation with easy management and storage of the long-lived highly radioactive nuclide compared to conventional UO_2 based fuels. The knowledge of basic thermodynamic properties of relatively new fuel materials is important for fuel design, performance modelling and assessment of safety issues. The fuel materials always possess inherent radioactivity. Therefore, experimental determination of thermodynamic properties requires extensive safety precautions and remote handling of samples. Hence, experiments can be performed in a limited temperature and/or composition range. Atomistic simulations can provide a gateway to predict thermodynamic properties of fuel materials in a wide temperature range. The first part of the talk will focus on evaluation of thermo-physical properties, viz., thermal expansion, thermal conductivity, melting temperature, superionic transitions, specific heats, density, elastic modulus, etc., of ThO_2 -rich $\text{Th}_{1-x}\text{Pu}_x\text{O}_2$ and $\text{Th}_{1-x}\text{U}_x\text{O}_2$ mixed oxides using atomistic simulations complementing experiments.

Burn-up of $(\text{U,Pu})\text{O}_2$ mixed oxide (MOX) fuels generates additional long-lived minor actinides (MAs) in the range of 0.1-1.0% yield. The Np and other MAs are a major concern for the storage of spent fuels due to their long-term radiotoxicity and heat generation in the spent fuel. ThO_2 -MAO₂ MOX are formed in a nuclear reactor from the transmutations of $(\text{Th,U})\text{O}_2$ and $(\text{Th,Pu})\text{O}_2$ MOX. Hence, a better understanding of UO_2 -NpO₂ and ThO_2 -NpO₂ pseudo-binary phase diagrams, including thermodynamic properties and electronic structures, are of interest in order to assess the stability domain of these materials. The study of phase equilibria in UO_2 -NpO₂ MOX is made more complex by non-collinear magnetic ordering in the ground state of NpO₂, UO_2 and their MOX. The formation of oxides of MA in the fuel affects the fuel behavior. Therefore, it is important to understand the thermodynamical and thermo-physical properties of $(\text{U,Np})\text{O}_2$ and $(\text{Th,Np})\text{O}_2$ MOX for better fuel performance.

The talk will also discuss the thermodynamic stability, phase diagram, thermal conductivity, oxygen diffusion and elastic properties of $(\text{U,Np})\text{O}_2$ and $(\text{Th,Np})\text{O}_2$ MOX and their effects on the fuel performance using the density functional theory and molecular dynamics based simulations.

Quantum Chemical and Molecular Dynamics Insights for the Extraction of Pharmaceutical moieties from aqueous environment Using Menthol-based Hydrophobic Eutectic Solvents

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The talk shall discuss Molecular Dynamics (MD) and Quantum Chemistry (QC) computations for pharmaceutical systems extracted from the aqueous medium. Distinct Deep Eutectic Solvents (DESs) consisting of DL-menthol as hydrogen bond acceptor (HBA) and carboxylic acids as hydrogen bond donors (HBDs) have been adopted as solvents. Using MD simulations, the non-bonded interaction energies along with the radial, combined, and spatial distribution functions were determined, highlighting the improved and beneficial interactions of DES components with pharmaceutical systems in comparison to water. In addition, transport parameters, such as the mean squared displacement and diffusivity of compounds within the phases, were analysed using Einstein's diffusivity equation in order to determine the affinity of the pharmaceutical moieties for the DES-rich phase. The simulation was used to calculate distribution coefficient, selectivity and extraction efficiency and were then compared with experimental liquid liquid equilibrium measurements. The charge-transfer procedure through QC confirmed the direction of charge transfer from DES to the pesticide, and the NBO analysis provided the stability of both DESs. This was confirmed by the structural findings of the MD simulation, which were initially validated by the experimental results.

Stabilization of Vaccinal RNA in D2O and Eliminating the Cold Chain

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To maximize their therapeutic activity, majority of the live vaccines are transported and stored at 2-8 °C. Maintenance of the optimal cold temperatures in the supply chain (“cold chain”) accounts for 80% of the financial cost of vaccination. To minimize this uneconomical and logistically challenging cold chain problem, we demonstrate that heavy water (D2O), in place of traditionally used H2O, is capable of stabilizing a labile vaccinal genome at a significantly high temperature. Structure tightening by D2O especially at a higher temperature is experimentally known for some time,¹ although molecular level understanding of this phenomenon is still lacking. Here using a combination of parallel tempering (PT) and metadynamics (MetaD) sampling methods, we first establish that D2O indeed imparts thermal stability to the native structure of a polio viral RNA hairpin (according to WHO’s immunization program, oral polio vaccine is the most thermo labile of all vaccines). Then we set out to investigate the molecular foundation of this finding by probing the hydration dynamics of the RNA, hydration shell around the RNA surface, and spatial dependence of RNA-solvent collective hydrogen bond (HB) dynamics in the THz domain.

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How Osmolytes balance surface charges under Salt-stress

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To counter stress of salt imbalance, cell often produces low molecular weight osmolytes to resuscitate homeostasis. However, how zwitterionic osmolytes would tune the electrostatic interactions among charged biomacromolecular surfaces under salt stress, has eluded mainstream investigations. Here, via combination of molecular simulation and experiment, we demonstrate that a set of zwitterionic osmolytes are able to restore the electrostatic interaction between two negatively charged surfaces that had been masked in presence of salt. Interestingly, the mechanisms of resurrecting charge interaction under excess salt are revealed to be mutually divergent and osmolyte-specific. In particular glycine is found to competitively desorb the salt-ions from the surface via its direct interaction with the surface. On the contrary, TMAO and betaine counter-act salt stress by retaining adsorbed cations but partially neutralising their charge-density via ion-mediated interaction. These access to alternative modes of osmolytic actions would provide the cell the required flexibility in combating salt-stress.

Predicting microstructures of polymer blends and composites using AI and molecular simulations

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Polymer blends and composites offer a broad range of thermophysical properties that are linked to their compositions. However, it is challenging to establish a universal composition-property relation of these systems due to their enormous composition and chemical space.

Here, we address this problem and develop a new method to model the composition-microstructure relation of polymer blends and composites through an intelligent machine learning pipeline named nanoNET. The nanoNET is a radial distribution function predictor, built upon computer vision and image recognition concepts. It integrates unsupervised deep learning and regression in a fully automated pipeline. We conduct coarse-grained molecular dynamics simulations of different class of polymer blends and composites; and utilize the data to establish and validate the nanoNET. Within this framework, a random forest regression model predicts the spatial distribution of chemical moieties in a binary system in a latent space. Subsequently, a convolutional neural network-based decoder converts the latent space representation to the actual radial distribution function of the chemical moieties of the binary system. The nanoNET predicts spatial correlation function for many unknown polymer nanocomposites and blends very accurately. This method is very generic and can accelerate the design, discovery, and fundamental understanding of composition-microstructure relations of polymer blends, composites and other molecular systems.

Atomistic Design and Decoding of Multi-component Glasses

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Fusion of valuable material properties has lent the acceptance of sodium borosilicate (NBS) glasses for nuclear waste immobilization. In spite of popularity, the mechanisms associated to these properties are yet only partially discovered and need further exploration. Considering that, the combinations of experiments, molecular dynamics (MD) simulations and models were used to understand the role of composition for various structural and physical aspects of vitrified borosilicate glasses. The extensive molecular dynamics simulations were performed to disclose the beneficial aspects of doping NBS glasses with TiO₂, BaO and ZnO. First principles ab-initio MD (AIMD) simulations confirmed the transferability of BKS potential model for multi-component glasses in MD simulations. The results capture significant amendment in short and intermediate range order parameters: bond/angle distribution profiles, structure factor and probability of X-O-X (X,X\ = Si, B, Zn, Ba, Ti) connections. Successively, the effect of microscopic structure on observable glass properties: chemical durability, mechanical strength, thermal stability and characteristic vibrational spectra was analyzed. Order of connectivity illustrated that hydrolysis of glass will slow down with addition of either of ZnO/BaO/TiO₂ in the NBS glass matrix. Low R (Na₂O/B₂O₃) and high K (SiO₂/B₂O₃) of doped sodium borosilicate glass surface compared to bare NBS represents the more stable structure of glass surface will be produced for doped-NBS than NBS. During contact with water, Na⁺ ions were less likely to leach out from glass to aqueous solution for doped NBS glasses. The enhanced chemical resistivity of doped NBS was also established from the increasing activation energy for diffusion of Na ions. Likewise, the ring statistics as well as Na cluster size also supported the reduced chemical reactivity of doped glasses. The systematic study of linkage between network formers, ring statistics, diffusion dynamics and ion/water migration provides significant understanding of glass dissolution mechanism. Also, results predict the beneficial impact of glass doping for improved strength of glass skeleton, which would eventually control the glass degradation due to micro cracking. The combined studies from experiments and MD simulations disclose many interesting microstructure and dynamics due to the presence of doped elements in the NBS glass matrix. The present talk will discuss about the design and engineering of multicomponent glass using MD simulations.

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