

7th Molecular Simulations Workshop Northeastern Regional Edition

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1 Invited Talks

1.1 Dr. Noam Bernstein Iterative Fine Tuning of MACE Foundation Models

U.S. Naval Research Laboratory, Center for Materials Physics and Technology

Abstract:

The MACE equivariant message-passing graph-neural-network machine-learning interatomic potential (MLIP) framework has enabled the development of pre-trained foundation models, fit to density-functional theory calculation of materials spanning essentially the entire periodic table [1, 2]. Taking advantage of the reasonable as-is accuracy of the foundation models, and multi-head stabilization of the fits, I describe a simple workflow for producing fine-tuned MACE models using an iterative molecular dynamics/fitting procedure. I show how this procedure produces potentials that are more accurate for specific systems. I give a few examples of the application of this approach to the temperature-composition phase diagram of a structural metallic alloy, proton diffusion in a solid electrolyte, and structure phase transitions in a tin-halide perovskite. I also describe the workflow scripts, which use the wfl python library [3] to automatically parallelize the molecular dynamics, DFT evaluation, and MACE fine tuning fit tasks, and present a VASP-like interface for controlling the simulations.

1. Batatia, I. et al. "A foundation model for atomistic materials chemistry." J. Chem. Phys. v. 163, p. 184110 (2025).
2. <https://github.com/ACEsuit/mace-foundations>
3. <https://github.com/libAtoms/workflow>

Bio:

Dr. Noam Bernstein got his Ph.D. from Harvard University in 1998, joined the U. S. Naval Research Laboratory (NRL) as an NRC postdoc in 1998, and stayed as research staff starting in 2000. Dr. Bernstein has over 130 publications, an h-index of 48, and is a Fellow of the American Physical Society. He has worked on a wide range of atomistic simulations of material properties, including mechanical and structural properties of solids ranging from structural metals to Li-ion battery electrolytes. To study these materials he applies methods ranging from first principles DFT to interatomic potentials using energy minimization, molecular dynamics, and free energy calculations. Most recently he has collaborated on the development and application of machine learning interatomic potentials, including the ground-breaking GAP formalism and the equivariant neural network MACE foundation models.

1.2 Prof. Ian Bourg Multiscale Simulation of Hydrated Clay Colloidal Assemblages

Princeton University, Civil and Environmental Engineering

Abstract:

Phyllosilicate minerals, a.k.a. clay minerals, are a key building block of soils, sediments, and sedimentary rocks. These charged nanoparticles have a high specific surface area and high aspect ratio and form complex aggregation structures that can retain large amounts of water and other substances, including organic compounds and contaminants. Their complex chemical and mechanical properties the resulting colloidal assemblages have implications across a wide range of applications, from soil carbon dynamics to contaminant fate and transport, soil resilience to erosion and drought, landslides and other geophysical hazards, high-level radioactive waste isolation, petroleum geology, civil engineering, and other areas. Detailed understanding of the complex properties of these materials requires examinations across different length scales and different physics. Here, we summarize our recent efforts to develop such understanding by combining molecular dynamics (MD), coarse grained (CG), and computational fluid dynamics (CFD) simulations of the coupled thermal, hydraulic, mechanical, and chemical (THMC) properties of clay colloidal assemblages.

Bio:

Ian Bourg is an Associate Professor in Civil and Environmental Engineering at Princeton University. His group studies the properties of water at interfaces, with a particular emphasis on the impact of clay minerals on subsur-

face hydrology, soil mechanics, carbon dynamics, geochemistry, and contaminant fate and transport. He obtained a B.Eng. in Industrial Process Engineering from the National Institute for Applied Sciences in Toulouse, France, in 1999 and a Ph.D. in Civil and Environmental Engineering from the University of California at Berkeley in 2004. He was a Research Scientist in the Earth Sciences Division at the Lawrence Berkeley National Laboratory (LBNL) before joining Princeton University in 2015.

1.3 Prof. Gregory Dignon

Phase Separation, Mixing and Demixing in Biomolecular Systems

Rutgers University, New Brunswick, Chemical and Biochemical Engineering

Abstract:

Biological compartmentalization is essential for life. While many compartments within a cell are bound by a lipid membrane, there are also many compartments which lack membranes and instead form through biomolecular phase separation. In this talk, we will consider two types of biomolecular systems that undergo liquid-liquid phase separation. The first involves the association or segregation of biological macromolecules such as proteins and nucleic acids into distinct regions known as condensates or membraneless organelles. We also consider systems involving lipid bilayers which form plasma membranes and organelle membranes, which undergo demixing to form lipid domains essential for biological function. In both cases, we consider the molecular properties and intermolecular interactions which allow for multiple regions of unique molecular compositions to coexist, rather than mixing into a single continuous phase. We utilize multiscale simulation and statistical physics to directly sample and characterize these systems.

Bio:

Prof. Dignon received his Bachelor's of Science in Chemical Engineering from Rensselaer Polytechnic Institute in 2015 where he conducted research with Prof. Pete Tessier. He then completed his PhD in 2019, studying under the advisement of Prof. Jeetain Mittal. He did his postdoctoral research under Prof. Ken Dill at Stony Brook University until starting as an Assistant Professor at Rutgers University in 2022. Prof. Dignon's lab uses molecular modeling, simulations, and statistical thermodynamics to study disordered biomolecular systems, including intrinsically disordered proteins, RNA structural heterogeneity, biomolecular condensates, and lipid membranes.

2 Posters

2.1 Aditya Dilip Lele, Development and Assessment of Curriculum Resources for Teaching Molecular Simulations and Their Applications

Rowan University

Authors: Aditya Dilip Lele; Kirti Yenkie; Gregory Santilli; Harriet Appiah; Andres Castellar-Freile; Ronald Borja-Roman; Robert Hesketh

Advances in computational resources as well as machine learning-based simulation techniques are poised to democratize the field of molecular simulations. Hence, there is arguably a greater need to incorporate the fundamentals of molecular simulations into undergraduate and graduate curricula across different engineering disciplines. In this poster, we present the online teaching resources developed for an interdisciplinary molecular simulations course at Rowan University. The course was taught to a group of 31 undergraduate and graduate students from Mechanical Engineering, Chemical Engineering, Biomedical Engineering, and Materials Science. We present a preliminary pedagogical assessment of the effectiveness of the course material on student learning outcomes. We also present a complementary set of teaching modules developed to teach environmental impact forecasting of chemicals and processes using molecular simulation, machine learning, and data analytics tools.

2.2 Diana Castaneda Bagatella, Sign-Consistent Curvature-Driven Surface Hopping for Robust Non-Adiabatic Dynamics

New Jersey Institute of Technology

Authors: Diana Castaneda-Bagatella; Dil Limbu; Farnaz Shakib

We present a methodological advancement in non-adiabatic molecular dynamics through the implementation and refinement of curvature-driven fewest switches surface hopping, coined as κ -FSSH, within our in-house SHARP software package. As the name suggest, curvature driven framework requires only adiabatic energies and gradients for dynamic propagation, thereby bypassing the explicit evaluation of derivative couplings and reducing the computational cost of non-adiabatic dynamics considerably. However, the method needs extensive benchmarking in different reaction regimes and environmental conditions to enter the mainstream of non-adiabatic dynamics simulations in condensed phases. With a systematic benchmarking against the Tully model systems, we identify a subtle but critical sign ambiguity in the calculated curvature-driven time-derivative coupling. While this issue has negligible impact in single avoided-crossing scenarios, it leads to qualitatively incorrect dynamics in multi-crossing systems. We introduce a physically motivated sign-consistency correction that restores the proper alternating structure of the coupling along nuclear trajectories without modifying its magnitude. This correction significantly improves the robustness and transferability of κ -FSSH. Finally, I will discuss how we extend both conventional FSSH and κ -FSSH to Liouville space by propagating the electronic density matrix rather than wavefunction amplitudes.

2.3 Egor Demidov, Is surface stress or surface free energy responsible for adsorption-induced deformation?

New Jersey Institute of Technology

Authors: Egor Demidov; Noam Bernstein; Gennady Gor

Adsorption-induced deformation (AID) is a well-known phenomenon of elastic expansion or shrinkage of materials caused by adsorption on their surfaces. Bangham's law is the widely-accepted explanation of AID. It attributes AID to decreasing surface free energy due to stabilization of the surface by adsorbate molecules. However, Bangham's law cannot explain adsorption-induced shrinkage observed in certain materials, since adsorption can only lower surface free energy, but cannot increase it. Recently, works have emerged that attribute AID to a related, but distinct quantity - surface stress. Seeking to resolve the confusion, we calculate the water-adsorption-induced change in both surface free energy and surface stress in a hydroxylated beta-cristobalite slab, which serves as a surrogate for amorphous silica. A Monte Carlo simulation with a machine-learning inter-atomic potential MACE-MH-1 is used to sample both quantities. Preliminary results have shown a consistency in the sign and trend between average surface stress and surface free energy. However, the individual components of surface stress can describe anisotropic deformation, which is a more physical description for many crystalline materials.

2.4 Geordy Jomon, Molecular Simulations of Organophosphorus Compounds: From Pure Species to Mixtures

New Jersey Institute of Technology

Authors: Geordy Jomon; Gennady Y. Gor

Understanding the properties of organophosphorous chemical warfare agents (CWA) is essential for its detection, decontamination, and destruction efforts. Due to its extreme toxicity, less toxic organophosphate molecules with similar physical structure have been used as CWA simulants in experimental studies. These simulants include dimethyl methylphosphonate (DMMP), diisopropyl methylphosphonate (DIMP), triethyl phosphate (TEP) etc. Molecular simulations routinely supplement the experimental efforts for simulants, and serve as an alternative to experiments for the actual agents. Monte Carlo and molecular dynamics simulations utilizing the united atom transferable potentials for phase equilibria (TraPPE) force field showed excellent predictions of various thermodynamic and transport properties of pure organophosphorus compounds [1, 2, 3, 4]. In reality, these organophosphates are rarely present as pure species in the environment, but rather as mixtures containing water or products of their decompositions, such as alcohols. The presence of these impurities even in a small concentration could have a significant impact on the thermodynamic and transport properties. In this work, we focus on molecular simulations of binary mixtures of TEP with water and methanol, using the published experimental data for comparison [5]. TEP and methanol are modeled using the TraPPE force field. We use the united atom representation for TraPPE, where CH_n groups are represented as a single interaction site. Simulations are performed using two water force field models—SPC/E and TIP4P/2005, to select the best model for interactions with TEP. We predict the excess volume and excess molar enthalpy of TEP-water and TEP-methanol mixtures at different concentrations using molecular dynamics simulations. Then, for selected concentrations, we study how the interactions between water and TEP affect the resulting viscosity.

Acknowledgment: This work was funded by the US Defense Threat Reduction Agency, through the University Research Alliance: Materials Science in Extreme Environments.

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2.5 Kaelyn Chang, Guiding Configurational Entropy Utilizing an Information-Theoretic Collective Variable

Rutgers New Brunswick

Authors: Kaelyn Chang; Ashley Z. Guo

Reinforcement learning can help accelerate the sampling of configurational pathways in molecular simulations. However, previous methods can be highly dependent on system-specific collective variables (CVs) in order to successfully sample towards a desired final configuration. Additionally, many previous works focus specifically on protein folding applications. This motivates a generalized collective variable that can guide a broader range of systems to target configurations in these learning algorithms. Here, we propose the computable information density (CID) as a more generalizable CV for sampling along a configurational pathway. In our previous work, we demonstrated CID as a practical CV that could capture differences in phase and morphology without a priori knowledge of ideal, system-specific order parameters. By utilizing a Monte Carlo Tree Search (MCTS), we set a target CID to explore from a metastable state to a stable one, which is then compared to an unguided control. We show that the CID-guided tree search not only reaches a specified target CID, but also produces more ordered and

energetically favorable configurations than its unguided counterpart. This establishes a foundation for information-theoretically guided, gradient-free optimization for sampling configurational pathways in a variety of molecular systems.

2.6 Mansi Gokani, Design considerations for polystyrene binding polypeptides

Rutgers New Brunswick

Authors: Mansi Gokani; Brianna Fea; Ashley Z. Guo

Plastic-binding polypeptides are an emerging class of materials with applications in nanoplastic capture, materials functionalization, and biosensor design. Polystyrene is a nanoplastic of particular importance; as a commodity plastic, its widespread use has led to it being a common contaminant in freshwater, posing a threat to environmental and human health. Peptide based materials may be leveraged to sequester polystyrene in water purification systems, but designing and evaluating polypeptides poses a new challenge. We use a computational workflow of atomistic molecular dynamics simulations and enhanced sampling to evaluate polypeptide binding to polystyrene. Resulting trajectories are processed to yield free energy calculations, analysis of the binding configurations, and an investigation of the solvation effects on the system. We find that binding to polystyrene is primarily mediated by cationic and aromatic residues such as arginine and tryptophan. However, these binding modalities rely on proper residue spacing; linking residues between bulky amino acids allow for more possible binding configurations. We also find that the presence of polypeptides shields the polystyrene from water, but it does not promote further self-collapse. Our analysis demonstrates that both sequence composition and sequence orientation are key considerations for designing a polypeptide with multiple binding modalities, identifying motifs in both cationic and aromatic enriched polypeptides that can be leveraged for future development of polystyrene binding polypeptides.

2.7 Margarita Gordiychuk, Searching for Sequence Features that Control DNA Cyclizability

Johns Hopkins University

Authors: Margarita Gordiychuk; Jonghan Park; Aakash Basu; Taekjip Ha; William Bialek; Yaojun Zhang

The mechanical properties of DNA molecules are crucial for many biological processes, from DNA packaging to transcription. While the mechanics of long DNA typically follow the worm-like chain polymer model, multiple studies have shown that the mechanics of short DNA, at the length scale of DNA-protein interactions, depend strongly on their sequence content. Motivated by recent high-throughput measurements of sequence-dependent DNA cyclizability – the DNA’s tendency to mechanically bend and form a loop – we developed a statistical-mechanics framework to systematically explore how cyclizability depends on the collective contributions of an increasing number of nucleotides in the sequence. By applying the method to datasets of randomly generated and biologically derived sequences, we identified a minimal pairwise model that describes the sequence-dependence of DNA cyclizability. The pairwise model enabled the extraction of characteristic sequence features that control DNA cyclizability and predicted the most and least cyclizable sequences, which we validated through all-atom molecular dynamics simulations.

2.8 Md Sojib Kaisar, Entropic Pressure in Confined Active Vesicles

New Jersey Institute of Technology

Authors: Md Sojib Kaisar; Rubayet Hassan; Fatemeh Ahmadpoor

Fluctuation-induced entropic forces play an important role in the mechanics and interactions of soft membranes. While entropic pressure in passive confined vesicles is well understood, the influence of active fluctuations on these interactions remains unresolved. Here, a theoretical framework is developed to quantify entropic pressure in confined active vesicles by extending Helfrich membrane mechanics to activity-driven fluctuations. A quasi-spherical vesicle is described using spherical harmonic modes, with activity incorporated through temporally correlated active forces and curvature-generating stresses. Analytical expressions are derived for the free energy, fluctuation amplitudes, and confinement-induced entropic pressure, revealing how activity alters both the magnitude and scaling of fluctuation-mediated forces, particularly through long-wavelength modes. The framework establishes a generalized mechanics-based description of activity-driven entropic interactions in curved membranes and provides predictive insight into membrane stability, vesicle interactions, and fluctuation-mediated phenomena in active biological and bioinspired systems.

2.9 Noor Aldin Alzghoul, Reactive Molecular Dynamics Investigation of Polyethylene Pyrolysis Under Rapid Thermal Conditions

Rowan University

Authors: Noor Aldin Alzghoul; Dr. Aditya Lele

Understanding and controlling reaction kinetics during polymer pyrolysis remains challenging due to the large number of possible reaction pathways, transient intermediates, and complex radical chemistry involved. Recent advances in pulsed Joule heating (PJH) have shown potential for improving product selectivity by controlling heating and reaction timescales compared with conventional pyrolysis; however, identifying suitable pulse conditions requires a better understanding of the relationship between temperature, reaction kinetics, and product evolution. In this work, ReaxFF reactive molecular dynamics simulations were used to investigate polyethylene pyrolysis and extract atomistic-level reaction mechanisms and kinetic trends without relying on predefined reaction pathways. The simulations capture the evolution of polymer decomposition, intermediate species, and the formation of light olefins, particularly ethylene (C_2H_4) and propylene (C_3H_6) under different thermal conditions. Temperature-dependent simulations were analyzed to determine the influence of temperature on reaction rates, product evolution, and characteristic formation timescales relevant to rapid thermal conversion processes. The kinetic insights obtained from the simulations guided experimental optimization and improved the combined light-olefin (C_2H_4 and C_3H_6) yield to approximately 47 %, while demonstrating how reactive molecular dynamics connects molecular-scale reaction behavior with experimentally relevant processing conditions for non-equilibrium polymer pyrolysis.

2.10 Ravindu L. Senevirathna, Molecular Dynamics of Nanobubble Nucleation in Water: Effect of PFAS on Nanoscale Cavity Formation

New Jersey Institute of Technology

Authors: Ravindu L. Senevirathna; Linda Cummings; Lou Kondic; Duwage Charitha Perera; Jay N. Meegoda

Ultrasound-induced acoustic cavitation involves the nucleation, growth, oscillation, and eventual collapse of nanobubbles (NBs) in liquids. It plays an important role in environmental remediation, sonochemistry, biomedical applications, and industrial processes. Despite extensive research on cavitation and NB dynamics, the molecular-scale mechanisms governing initial NB nucleation remain insufficiently understood. In particular, the influence of dissolved contaminants and surface-active species on the earliest stages of nucleation requires further investigation. In this work, molecular dynamics (MD) simulations investigate NB nucleation in water under tensile conditions and determine how perfluorooctanoic acid (PFOA) modifies nucleation behavior. In the present gas-free MD systems, the initial nucleation event is represented by the formation of a nanoscale low-density cavity in stretched water, which serves as the molecular-scale precursor to NB formation. We first investigated a pure-water system to establish a homogeneous nucleation baseline, and then a system containing neutral PFOA to evaluate the influence of per- and polyfluoroalkyl substances (PFAS) on cavity formation. We performed the simulations in periodic $2.5 \times 2.5 \times 2.5$ nm cells at 300 K, using TIP4P/2005 for water and OPLS-AA for PFOA. After system minimization and NVT and NPT equilibration, we generated hydrostatic tension through controlled, incremental isotropic expansion of the simulation cell. We performed NVT relaxation after each stretching increment. We developed a quantitative, equilibrium-calibrated cavity-detection methodology to distinguish persistent nanoscale cavities from transient intermolecular free-volume fluctuations. We further extended the analysis to characterize cavity persistence, morphology, and spatial association with PFOA. In pure water system, we identified a fully persistent cavity at approximately 3.66 % cumulative linear strain and a mean pressure of -187 MPa. In the neutral-PFOA system, persistent cavity formation occurred earlier, at approximately 3.15 % strain and -154 MPa. Thus, under the applied simulation conditions and persistence criterion, neutral PFOA shifted the onset of persistent cavity formation by about 33 MPa toward less negative pressure. The spatial analysis further showed that growing cavities became increasingly associated with the PFOA molecule as cavity size increased. Although smaller cavities showed an apparent preference for the fluorinated region of PFOA, the current results do not establish an exclusively tail-localized nucleation mechanism. These results demonstrate an MD framework for resolving the molecular-scale onset of NB nucleation under tensile conditions and indicate that neutral PFOA can facilitate nanoscale cavity formation relative to pure water. The framework provides a basis for further investigation of how PFAS chemistry, ionization state, concentration, and other molecular-scale heterogeneities influence NB nucleation and acoustic cavitation inception.

2.11 Rubayet Hassan, A Computational Model of Fluctuating Active Membranes: Implication for Entropic Pressure

New Jersey Institute of Technology

Authors: Rubayet Hassan; Fatemeh Ahmadpoor

Entropic forces generated by suppressed membrane fluctuations play a central role in interactions and stability of soft active matter systems. While entropic pressure in confined passive membranes is well understood, how nonequilibrium activity modifies confinement-induced entropic forces remains largely unexplored. In this work, we develop a computational framework to investigate the entropic pressure of confined fluctuating active membranes. The membrane is modeled as a solvent-free one-particle-thick elastic surface, where activity is introduced through localized oscillatory direct forces and curvature-generating spontaneous curvature patches, while confinement is imposed by two parallel hard walls that restrict membrane undulations. Using coarse-grained molecular dynamics simulations in LAMMPS, we quantify how active fluctuations modify the fluctuation spectrum and the resulting entropic pressure generated by confinement. Simulations show that activity amplifies long-wavelength fluctuations and significantly alters the scaling behavior of confinement-induced entropic pressure relative to passive membranes. In highly active regimes, deviations from classical equilibrium scaling emerge, revealing how activity modifies fluctuation-mediated repulsive forces. This study establishes a predictive framework for understanding fluctuation-mediated interactions in active membranes and vesicles, with relevance to biological processes such as vesicle fusion, intracellular transport, and the design of synthetic membrane systems with tunable entropic forces.

2.12 Sandip Bhusal, Ring Polymer Liouville Equation: A Robust and Efficient Approach to Non-Adiabatic Dynamics

New Jersey Institute of Technology

Authors: Sandip Bhusal

Mixed quantum-classical Liouville dynamics provides a rigorous framework for condensed-phase non-adiabatic simulations. However, its Wigner-sampled formulation converges slowly and exhibits qualitative failures at low temperature and under strong coupling. To address these limitations, the ring polymer Liouville equation (RPLE) is introduced, incorporating nuclear quantum effects into the bath mode via imaginary-time path integrals. Building on the surface-hopping solution of the quantum-classical Liouville equation (QCLE) using sequential short-time propagation, RPLE propagates the classical degrees of freedom as ring polymers, evaluates non-adiabatic transitions at the centroid level, and accumulates observables with a centroid-basis-projected, bead-averaged estimator. Benchmarking against QCLE for the spin-boson model across reaction regimes, coupling strengths, and temperatures shows that RPLE is accurate and robust, converging with one to four orders of magnitude fewer trajectories than QCLE. In the low-temperature and strong-coupling regime where QCLE fails, RPLE with 32 beads remains stable and yields physically meaningful population dynamics. Expanding the classical phase space with a ring polymer framework thus establishes quantum-classical Liouville dynamics as a practical and widely applicable tool for non-adiabatic condensed-phase simulations.

2.13 Santiago Flores Roman, MezCal: An Efficient Monte Carlo Simulation Software for Dense and Nanoconfined Fluids

New Jersey Institute of Technology

Authors: Santiago Flores Roman; Gennady Gor

The use of Monte Carlo (MC) simulations in the field of adsorption offers distinct advantages. By randomly sampling equilibrated system configurations and relating system behavior to infinite reservoirs, schemes such as grand canonical MC (GCMC) enable accurate, efficient thermodynamic predictions of confined fluids. However, standard MC modeling faces computational bottlenecks for dense systems. Alternative methods can overcome this limitation, such as extended equations of state for adsorbed systems or self-consistent methods (e.g., classical density functional theory) [1, 2]. While these methods remain efficient regardless of fluid density, they still require prior knowledge of the chemical potential and rely heavily on equations of state. For MC simulations, several methods have been proposed to improve configurational sampling efficiency. For example, insertion and deletion schemes for virtual particles (such as the Bennett acceptance ratio [BAR]) and finite-reservoir methods (such as mesocanonical ensemble MC [MCEMC]) have proven effective for predicting chemical potentials [3, 4]. For fluid density, configurational bias schemes were proposed, such as the configurational fractional component MC

(CFCMC) method, to improve configurational sampling efficiency [5]. Multiple MC programs have been developed to facilitate the modeling of a number of systems and predict their physical properties using the methods mentioned above. RASPA, Chainbuild, and Cassandra are a few examples [6, 7, 8]. In this work, we developed MezCal (mesoporous calculations), an open-source, intuitive, MC simulation engine specifically engineered for fluid confinement in implicit nanopores. MezCal provides highly accurate, on-the-fly chemical potential predictions regardless of fluid density and incorporates CFCMC moves to smoothly scale particle interactions in dense, confined fluids. We demonstrate the capabilities of MezCal by modeling liquid gallium—a highly dense fluid that typically causes conventional MC software to fail—confined within cylindrical silica pores ranging from 20 Å to 80 Å at 500 K, across a pressure range from ambient to 5 GPa. MezCal successfully predicted chemical potentials, isotherms, and isothermal bulk moduli of both bulk and confined gallium. The simulations showed that the density and stiffness of gallium decrease under confinement compared to the bulk phase due to the solvophobicity of the pores. This work provided new insights into the physical behavior of bulk and confined gallium and proposed a new MC engine capable of modeling dense systems in nanopores.

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2.14 Shahid Akbar, From 2D to 3D designing of Electrically Conductive and Magnetically Bi-stable Coordination Polymers

New Jersey Institute of Technology

Authors: Shahid Akbar; Shogo Nakaza; Farnaz Shakib

Magnetically bi-stable conjugated coordination polymers (bi-CCPs) are a new class of hybrid organic-inorganic CCPs that can undergo transitions between different magnetically disparate spin states, i.e. spin crossover (SCO) induced by external stimuli. Equipping these bi-CCPs with an inherently high electrical conductivity will allow the use of electric current to track the spin transition, realizing a "dream" nano-scale sensing material. The synthetic versatility (compositional and electronic tunability via ligand and metal modifications) and different topologies of bi-CCPs offer inverse engineering opportunities for inducing high electrical conductivity. Incorporating high electrical conductivity in SCO materials has been a challenging and somewhat overlooked task, with most reported bi-CCPs to date being insulators. Here, we propose to use atomistic-level calculations at the periodic density-functional theory (DFT) level to provide a fundamental molecular-level understanding and control of the interrelation between electronic spin-states and lattice dynamical properties, as well as electrical conductivity and the SCO phenomenon. We will then use the produced insights into the structure-property-function relationship of known bi-CCPs to guide the rational design of new classes of bi-CCPs via pillar-ligand insertions in recently introduced 2D-layered electrically conductive (EC) pi-stacked MOFs. We will create a comprehensive database of hypothetical 3D EC bi-CCPs. Once generated, these hypothetical structures will be evaluated using an automated high throughput screening (HTS) workflow utilizing MACE (a Machine-learned Interatomic Potential) to quickly analyze a large number of bi-CCPs for their thermodynamic stability, structural features and electrical conductivity. This HTS setup will filter a large number of structures to select structures with high electrical conductivity, high carrier mobility, and discrete magnetic properties of different spin states will be suggested for experimental synthesis. Collectively, this will lay the foundation for future theoretical and experimental research in the field of next generation EC bi-CCPs.

2.15 Shannon Zhang, Asymmetric Effects Underlying Dynamic Heterogeneity in Miscible Blends of Poly(methyl methacrylate) with Poly(ethylene oxide)

Princeton University

Authors: Shannon Zhang; Michael A. Webb

The emergence of spatially variable local dynamics, or dynamic heterogeneity, is common in multicomponent polymer systems. Although often attributed to differences in the intrinsic dynamics of each component, the molecular origin of their coupling and its dependencies remain unclear. Here, we use molecular dynamics simulations of poly(ethylene oxide) (PEO)/poly(methyl methacrylate) (PMMA) blends, across the full range of compositions and multiple thermal regimes, to characterize local fluctuations and subchain relaxations for both PEO and PMMA. By constructing probability distributions of local composition and computing entropic measures, we connect nanoscale heterogeneity to differences in mobility between PEO and PMMA, extending beyond mean-field treatments. While PMMA segmental fluctuations in blends broadly align with T_g-equivalent neat PMMA systems, PEO exhibits enhanced mobility correlated with increased free volume and broader, more diverse local compositions upon blending. Rouse-mode analysis, used to probe relaxation dynamics over different length scales, shows that PEO relaxation approaches neat-like behavior in PEO-rich domains, whereas PMMA relaxation accelerates uniformly across all mode numbers. Given the local mobility enhancement of PMMA by PEO, this uniform shift suggests a nanoscale facilitation process that extends PEO's influence beyond its immediate environment. These findings link the statistics of local compositional heterogeneity to dynamic asymmetry across length scales, provide physical insight into the behavior of this archetypal blend system, and establish a framework for analyzing dynamic coupling in others.

2.16 Shogo Nakaza, Exploring 2D metal-organic frameworks as next generation Li and Na-ion cathode materials

New Jersey Institute of Technology

Authors: Shogo Nakaza; Shahid Akbar; Farnaz Shakib

Lithium ion batteries widely used today have several limitations including their flammable liquid electrolyte and degradability, making alternative battery options an attractive field of study. One promising alternative is solid state batteries with much higher energy density, faster charging, and safer components. 2D electrically conductive metal-organic frameworks (EC MOFs) are excellent potential cathode materials for this purpose as they provide high conductivity along with large surface area, and accessible redox active sites, i.e., both metal centers and organic ligands. In order to explore their potential, we are developing a 2D MOF-based solid-state battery cathode database. High throughput screening of the new database can identify promising candidates for battery applications. We implement a pymatgen-based lithium and sodium insertion workflow with a focus on 2D MOFs in our already existing and publically available EC MOF Database. The workflow takes a relaxed MOF structure and finds candidate ion insertion sites using the charge density. The inserted structures are optimized at the periodic density functional theory (DFT) level and the most stable structure is selected for the next round of insertion. The insertions are continued until the structure is no longer topotactically stable. This workflow provides detailed information on adsorption energy and voltage of the possible cathode materials.

2.17 Sowmya Atukuri, Mechanistic Investigation of Nanobubble-Assisted Water Washing for Enhanced Oil Removal from Contaminated Soil

New Jersey Institute of Technology

Authors: Sowmya Atukuri; Wen Zhang

Oil contamination of soil remains a significant environmental challenge, requiring efficient and sustainable remediation technologies. This study investigates the application of nanobubble-assisted water washing for enhanced oil removal from contaminated soil and elucidates the underlying mechanisms. Different gaseous nanobubbles were generated and characterized, exhibiting bubble diameters of 100–300 nm and a CO₂ nanobubble zeta potential of -13.4 ± 0.5 mV. Laboratory experiments demonstrated that nanobubble water significantly improved the detachment and mobilization of oil from contaminated soil, achieving nearly 100 % oil removal, whereas conventional deionized water showed substantially lower removal efficiency. Nanobubbles also increased gasoline dispersion in water by more than 2.5-fold compared with DI water. Mechanistic investigations involving nanobubble partitioning, viscosity, surface and interfacial tension, and surfactant effects revealed that enhanced oil removal resulted from improved nanobubble–oil interactions, increased oil dispersion, and modified interfacial properties. These findings demonstrate the potential of nanobubble water washing as an efficient and environmentally sustainable technology

for remediation of oil-contaminated soils while providing new insights into nanobubble transport and interfacial mechanisms.

2.18 Trinh Quoc Dat Luong, Mechanical Properties of Necks Between Primary Spheres in Carbonaceous Aggregates: A Molecular Dynamics Study

New Jersey Institute of Technology

Authors: Trinh Quoc Dat Luong; Egor Demidov; Alexei Khalizov; Gennady Gor

Soot aggregates are fractal structures composed of carbonaceous primary particles held together by solid necks. On a microscopic level, the carbonaceous material is a composite of amorphous and graphitic carbon, with the degree of graphitization dependent on combustion conditions under which the aggregate was formed. During the atmospheric lifetime of soot, initially fractal aggregates undergo compaction driven by surface tension of condensed liquid coatings. Changes in morphology of soot aggregates affect their climate forcing properties and are widely studied. Formation conditions control the mechanical strength of aggregates through their microstructure, and therefore have an indirect impact on the evolution of aggregate morphology in the atmosphere. Using molecular dynamics, we derive mechanical properties of necks between primary particles in soot aggregates with microstructures that correspond to different combustion conditions. Composite necks, which form in recirculating flames, and fully graphitic necks, which are more likely to form in non-recirculating flames, were deformed to failure in tension and in shear. Elastic moduli and yield strengths were derived. The produced set of parameters is ready to use with a soot mechanics model previously developed by our group. Through the mechanics model, it is now possible to investigate the effects of formation conditions of soot on the outcome of coating-induced compaction numerically.

2.19 Tyler Oberholtzer, Comparative Molecular Dynamics Simulation of Oxygen Nanobubble Behavior Using GROMACS and LAMMPS

New Jersey Institute of Technology

Authors: Tyler Oberholtzer; Duwage Perera; Jay Meegoda

Sonolysis is an emerging technology which utilizes ultrasonic waves to form and collapse microbubbles at extremely high temperatures, enough to fully mineralize PFAS (per- and polyfluoroalkyl substances) molecules in water systems. However, this technology is limited by our current understanding of micro- and nanobubble physics, which prohibits the development of large-scale industrial remediation systems. Molecular Dynamics (MD) simulations provide a means of investigating this behavior at the molecular level, enabling the study of nanobubble physics at a scale that is difficult to resolve experimentally. However, the accuracy and reproducibility of MD simulation results can depend on the software, algorithms, and numerical implementations used. GROMACS and LAMMPS, two widely accessible MD platforms, have been used by researchers to explore complex molecular systems, including nanobubbles, but they employ different computational systems, which can result in conflicting simulation results. Comparing their ability to model oxygen nanobubbles under identical conditions can help determine whether observed nanobubble behaviors are consistent across platforms or sensitive to the computational methodology. This study therefore aims to construct and analyze oxygen nanobubbles using both GROMACS and LAMMPS. Parameters such as O_2 dissolution, nanobubble radius, and internal pressure will be compared to the Young-Laplace and Epstein-Plesset equations to assess the agreement between these two platforms. Our current efforts have revealed that GROMACS experiences an increase in O_2 dissolution, internal pressure, and radius decay compared to LAMMPS. We have also found that GROMACS permits water molecules to diffuse into the nanobubble region, a phenomenon not observed in LAMMPS. Future work will investigate the exact mechanisms that cause these changes, methods of equating simulation results across platforms, and scaling to larger systems ($r > 50\text{nm}$).

2.20 Udochukwu Laura Nwanebu, Density Functional Theory Study of pH-Dependent Short-Chain PFAS Adsorption on Kaolinite and Montmorillonite Basal and Reactive-Edge Surfaces

New Jersey Institute of Technology

Authors: Udochukwu Laura Nwanebu; Duwage Perera; David Washington; Jay Meegoda

Per- and polyfluoroalkyl substances (PFAS), the persistent "forever chemicals," accumulate in soils and groundwater, making it critical to understand how they bind to the clay minerals that govern their transport. We present

a periodic density functional theory study (Quantum ESPRESSO; PBE with Grimme-D3 dispersion) of two short-chain PFAS, perfluorobutanoic acid (PFBA) and perfluorobutanesulfonic acid (PFBS), on kaolinite and montmorillonite. On the basal faces, sulfonate binds more strongly than carboxylate on kaolinite (-73.9 vs -67.5 kJ/mol, flat orientation), and both prefer lying flat; this preference inverts on montmorillonite, showing that head-group selectivity is mineral-dependent. We further examine kaolinite reactive edges across three protonation (pH) states. Preliminary results reveal a pH-dependent trend: binding strengthens from acidic to basic edges, with a switch in molecular selectivity driven by a shift from charge-dominated to hydrogen-bond-dominated interactions. These findings identify surface protonation as a tunable control on PFAS retention, relevant to clay-based remediation. Ongoing work incorporates aqueous solvation for environmentally realistic conditions.

2.21 Vid Liam Stijelja, A Comparative Study on Effects of Defects on Thermal Conductivity in Silicon

Rowan University

Authors: Vid Liam Stijelja; Eddie Tang; Prithvi Ravi; Amin Nozariasbmarz; Aditya Dilip Lele

Controlling lattice thermal conductivity independently of electrical conductivity is important in the design of thermoelectrics and thermal management materials, and defect engineering is a viable way to gaining that control. A systematic ranking and direct comparison across these distinct defect classes remains under-explored. Using equilibrium molecular dynamics with the Green-Kubo formalism, we compare how vacancies, substitutional impurities, interstitials, and extended void defects modulate the lattice thermal conductivity of crystalline Si and Ge across different defect concentrations and temperatures. Point defects suppress thermal conductivity more than extended voids with the same number of atoms, with vacancies and interstitials being the strongest and substitutions and voids the weakest. The suppression is exponential in concentration for both materials. The ranking is itself concentration dependent, with variance being highest at lower levels and minimal at higher fractions between point-defect classes. Phonon density-of-states and strain analyses attribute these trends to the combined action of mass contrast, local bonding rearrangement, and strain rather than distortion alone. The framework established here characterizes each defect class in isolation, yet silicon rarely contains only one. Further work is currently extending this to multi-defect regimes, specifically evaluating the accuracy limits of Matthiessen's rule in silicon. The rule is an approximation assuming independent scattering additivity. Preliminary results indicate well-defined breakdown regimes, which will be presented along with potential underlying mechanisms.

2.22 Vladimir Grigorev, Mesoscale Heterogeneity Shapes Molecular Selectivity and Transport in Biomolecular Condensates

Johns Hopkins University

Authors: Vladimir Grigorev; Yaojun Zhang

Growing experimental and computational evidence suggests that many condensates exhibit heterogeneous internal organization at mesoscopic length scales. How such mesoscale organization influences client selectivity and transport, however, remains poorly understood. Here, we use coarse-grained molecular dynamics simulations to compare homogeneous and heterogeneous sticker-spacer condensates with matched scaffold density, sticker fraction, and sticker-sticker interaction strength. We find that the two condensates exhibit markedly different client partitioning profiles and transport dynamics. In the heterogeneous condensate, clients sample distinct local microenvironments in a size-dependent manner, leading to pronounced differences in their transfer free energy compared with the homogeneous condensate. The heterogeneous internal organization also generates local environments with different mobilities and constraints, giving rise to transient subdiffusion and non-Gaussian displacement distributions in client motion. Our results identify mesoscale organization as an important physical factor controlling both molecular selectivity and transport in biomolecular condensates, with implications for the biochemical functions of both natural and engineered systems.