6th Molecular Simulations Workshop
Northeastern Regional Edition

Contents

1 Invited Talks

1.1 Prof. Adib Samin
On the Degradation of Alloys: Insights from Multi-scale Simulations

Air Force Institute of Technology

Abstract:
With the technological advances of the past century, there is an increasing demand for reliable materials to operate in a variety of extreme and harsh environments including high stresses, elevated temperatures, oxidizing environments, and radiation damage. From phase diagrams, to thermal, mechanical, and kinetic properties, first principles-based calculations and atomistic simulations may significantly aid with the materials discovery process, elucidate unknown quantities or mechanisms, and inform our understanding of material response in extreme environments. In this talk, I will outline some recent examples of how atomistic simulations simulations may be effectively utilized to inform our knowledge regarding the behavior of materials in these extreme environments. I will specifically discuss examples concerning dislocations in binary alloys and the effect of segregation, the impact of defects on shock propagation, fracture and the effect local atomic environment surrounding grain boundaries, and the high temperature oxidation of multicomponent alloys.

Bio:
Dr. Adib Samin is currently an associate professor within the engineering physics department at the Air Force Institute of Technology (AFIT). Dr. Samin obtained his graduate degrees in chemical physics and mechanical engineering at the Ohio State University and performed research investigating radiation damage on magnets. During his postdoctoral years, Dr. Samin worked on the recycling of spent nuclear fuel, surface electrochemistry, and corrosion before joining Los Alamos National Laboratory as a Director's fellow working on modeling structural materials relevant to nuclear reactors. Dr. Samin is also the recipient of the Air Force 2024 Arthur Fleming Award in the basic science category.

1.2 Prof. Thomas E. Gartner III
Simulating Supercooled Water and Ice Polymorphs from Machine Learning Potentials

Lehigh University

Abstract:
Over the past 50 years, molecular simulations have emerged as a key tool to predict and understand how the molecular level features of a molecule (e.g., chemistry, size, topology, composition) combine with processing approaches (e.g., heat, flow, solvents, surfaces/interfaces) to control the structure and properties of fluids and soft matter. To produce useful insights, one must choose the right models and simulation protocols that capture the key physics of the system of interest within a reasonable computational cost. This choice can be particularly challenging in the context of soft matter, as capturing both angstrom-scale chemical detail and nm-to-micron- scale collective assembly processes is often necessary for a complete description of the material's structure and properties. In this talk, I will discuss how recent advances in machine learning (ML)-based simulation methods are changing the paradigm of molecular modeling in this context. Now, we have access to methods with predictive capabilities comparable to ab initio quantum chemistry approaches, but at speeds compatible with the long time and length scales needed to capture complex collective behavior. These advances allow us to provide important physical insights even when experimental data is scarce or incomplete. To illustrate these advantages, I will discuss the application of ML-based simulation methods to better understand the properties and phase behavior of water. We developed a neural network model to describe water's potential energy surface as obtained from density functional theory calculations, and then used state-of-the-art enhanced sampling techniques to show first-principles evidence for water's second critical point, a difficult-to-study phenomenon that may help explain water's anomalous thermophysical properties. From there, we applied this model to study the depressurization- induced melting of different ice crystal polymorphs and helped clarify the relationship between the complex melting behavior of ice polymorphs to water's liquid-liquid transition.

Bio:
Thomas E. Gartner III is an Assistant Professor in the Department of Chemical and Biomolecular Engineering at Lehigh University. His research group develops advanced computational approaches to understand and predict the structure and thermodynamics of polymers and soft materials for energy, sustainability, and technology applications. Gartner joined Lehigh in August 2023, and was previously an Assistant Professor in the School of Chemical & Biomolecular Engineering at the Georgia Institute of Technology. His awards and honors include the Dolores T. and William E. Schiesser Faculty Fellowship, the Stabler Award for Excellence in Teaching from Lehigh University, and selection as a DARPA Riser in the 2022 DARPA Forward conference series.

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1.3 Prof. William Jacobs
Nonequilibrium Dynamics at Biomolecular Condensate Interfaces

Princeton University

Abstract:
Interfacial properties play important roles governing the nucleation, fusion, and coarsening of phase-separated droplets. In the case of intracellular biomolecular condensates, these properties can be influenced by nonequilibrium processes, which are ubiquitous within living cells. I will discuss how steady-state chemical reactions modify the interfacial properties of biomolecular condensates and thus fundamentally alter the dynamics of intracellular phase separation. I will first introduce a molecular-level theory to quantitatively predict the interplay among reactive and diffusive fluxes near condensate interfaces. I will then show that steady-state chemical reactions can substantially alter interfacial fluctuations, producing a nonequilibrium surface tension that can be measured in molecular simulations. These results point to novel mechanisms for controlling the dynamics of phase separation within living cells, and also highlight the importance of considering nonequilibrium interfacial phenomena in the development of quantitative models of biomolecular condensation.

Bio:
William Jacobs obtained a B.S. in Physics and Engineering Science from the University of Virginia in 2010 and a Ph.D. in Theoretical Chemistry from the University of Cambridge in 2014. After completing a postdoc in Theoretical Chemistry and Biophysics at Harvard University, he began his independent career at Princeton University in 2019, where he is also affiliated with the department of Chemical and Biological Engineering, the Princeton Materials Institute, and the Biophysics program.

2 Posters

2.1 Alina Emelianova, Prediction of small-molecule partitioning into biomolecular condensates from simulation

Princeton University
Authors: Alina Emelianova; Pablo L. Garcia; Daniel Tan; Jerelle A. Joseph

Predicting small-molecule partitioning into biomolecular condensates is the key to developing drugs that selectively target aberrant condensates. However, the molecular mechanisms underlying small-molecule partitioning remain largely unknown. Here, we first exploit atomistic molecular dynamics simulations of model condensates to elucidate the physicochemical rules governing small-molecule partitioning. We find that while hydrophobicity is a key factor in determining partitioning into condensates enriched in hydrophobic residues, partitioning into more polar condensates is driven by specific interactions that can offset the associated entropic cost of localization. The observed selectivity of condensates toward certain compounds suggests that condensate-specific therapeutics can be engineered. Building on these insights, we develop minimal models (MAPPS) for the efficient prediction of small-molecule partitioning into biologically relevant condensates. We demonstrate that this approach reproduces atomistic partition coefficients in both model systems and condensates composed of the low-complexity domain (LCD) of FUS. Applying MAPPS to various LCD-based condensates shows that the protein sequence can exert a selective pressure, thereby influencing small-molecule partitioning. Collectively, our findings reveal that partitioning is driven by both small molecule–protein affinity and the complex interplay between the physicochemical properties of the compounds and the condensate environment.

2.2 Bicha Azizova, Simulating Catalytic Depolymerization of Polyolefins

Lehigh University
Authors: Bicha Azizova; Thomas E. Gartner III

Plastics depolymerization is a possible approach to reintegrate plastic waste into new chemical products, providing opportunities for waste minimization. Catalytic depolymerization of polymers enables control over downstream products, but a comprehensive picture of polymer chain configurations and transport near catalytic surfaces is largely missing, which would inform the design and control of depolymerization processes. In this work, we use classical molecular dynamics simulations to investigate the structure of polyolefin melts in contact with platinum surfaces. We characterize the effects of temperature, catalytic surface structure, and molecular weight on the intra- and intermolecular ordering of polyethylene chains near the surface. First, we evaluated possible force fields by comparing the adsorption energy of carbon atoms on the Pt surface. Using the OPLS-L and UFF models, we obtained an adsorption energy of 0.07 eV per carbon, in good agreement with experimental results for n-alkane molecules. Furthermore, the orientation order parameter confirms that Pt(100) induces strong ordering in the adsorbed polyethylene segments. These results may allow us to rationalize trends in molecular weight distributions of catalytic hydrogenation products and design more effective polymer-catalyst systems.

2.3 Christian Randolph, Expanding polymer integral equation theory with ML

Lehigh University
Authors: Christian Randolph; Thomas E. Gartner III

Integral equation theory provides a theoretical framework for calculating the thermodynamic quantities of isotropic liquid and liquid-like systems. The Polymer Reference Interaction Site Model [1] extends the original Ornstein-Zernike equations to polymer systems and allows for the calculation of critical thermodynamic quantities magnitudes faster than analysis from traditional Molecular Dynamics (MD) simulations. For these calculations, PRISM equations require closure relations that are a field of continuous research to increase the accuracy of calculations. New Machine Learning (ML) tools have provided an opportunity to efficiently develop data-driven closures for a range of polymer systems. A new ML closure for homopolymer systems has been developed that is more accurate in its calculations than the classical Percus-Yevick closure. Initial results agree with analysis from MD simulations as well as small-angle neutron scattering experimental data. Future work will include the development of ML closures that extend to more complex systems such as polymer blends, copolymers, and other experimental data.

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2.4 Daniel Mottern, Computational Investigation of Perfluoroalkyl Substance Adsorption in 3-Dimensional Covalent Organic Frameworks

New Jersey Institute of Technology
Authors: Daniel D. Mottern; Andrei L. Kolesnikov; Gennady Y. Gor; Joshua Young

Recent concerns over the accumulation of per- and poly-fluoroalkyl substances (PFAS) in surface and groundwater sources have stimulated research into novel porous materials for selective PFAS adsorption. Covalent-organic frameworks (COFs) represent one of he promising families of materials for this application. Here, we investigated the effects of the chemistry and structure of COFs on the adsorption of perfluorooctanoic acid (PFOA), a commonly seen PFAS molecule. Through Monte Carlo (MC) simulations, we found that nitrogen-based COFs tend to show high potential for PFAS adsorption. We also see that the void fraction of the COF pores have a significant effect on PFOA adsorption, with higher void fractions exhibiting lower potential for PFAS adsorption than those with moderate void fractions. We additionally investigated the effects of COF functionalization with -CF3 and -NH2 functional groups, showing that both functional groups strengthen interactions between the PFOA molecule and COF, but may decrease the porosity needed for effective adsorption of PFOA. For COFs with large enough pores, the addition of these functional groups can greatly improve the adsorption of PFOA, and could allow for the effective capture of PFAS from aqueous environments.

2.5 Egor Demidov, Chemisorption-induced surface stress in hydroxylated silica

New Jersey Institute of Technology
Authors: Egor Demidov; Andrei Kolesnikov; Gennady Gor; Alexei Khalizov

Adsorption-induced deformation is the expansion or contraction of a solid upon adsorption on its surface. It plays an important role in the properties of materials with a large surface area, such as porous materials. Adsorption-induced deformation is driven by surface stress in the solid, which is caused by adsorption. Utilizing molecular dynamics simulations, we compute surface stress in quartz induced by hydroxylation of the surface, a type of chemisorption, and submergence of the surface in water. Additionally, we compute surface free energy of quartz surfaces under different conditions using the Einstein crystal method.

2.6 Ethan Fisher, Molecular Mixed Metal-oxo Clusters: Well-defined Models for Mixed-Metal Oxide Nanomaterials

University of Florida
Authors: Ethan G. Fisher; Khalil A. Abboud; George Christou

Metal oxides such as CeO2 and Bi2O3 are employed in various applications spanning environmental remediation, sustainable energy development, and medicine. While effective, there remains ongoing debate regarding various material properties and mechanisms-of-action due to the inherent limitations of traditional nanoparticle syntheses (such as the range of sizes and shapes in any given batch) and characterization techniques (such as limited resolution). In contrast, the complementary 'bottom-up' approach can yield molecular metal-oxo clusters, which are identical in size and shape and adopt the same structure as the bulk solid; they therefore represent ultra-small (1–3 nm), atomically-precise pieces of the latter. As such, the so-called "molecular nanoparticles" enable a robust experimental and computational investigation into critical material properties and the establishment of synthesis-structure-property-performance relationships with atomic precision. Once characterized, comparisons and contrasts with the traditional nanomaterials can also be explored. Recently, interest in mixed-metal oxide nanomaterials has exploded owing to their enhanced properties, often arising from the synergistic interactions between each component in the bulk or at interfaces between different phases. For example, Ti/CeO2 shows promise as a photoanode for water splitting under visible light, and Cu/Bi2O3 is being investigated as a photo/electrocatalytic material for the reduction of CO2. While these mixed-metal oxides often display several enhancements over those of the individual binary metal oxides, their mixed-metal nature also increases their complexity, further limiting our ability to characterize them to atomic resolution. Herein, we describe the successful extension of our 'molecular nanoparticle' approach to various unprecedented molecular Ce/Ti-oxo and Bi/Cu-oxo clusters, and their characterization as well-defined models for the analogous mixed-metal oxide nanomaterials. These examples will further emphasize the advantages, benefits, and potential universality of the molecular approach to ultra-small nanomaterials.

2.7 Geordy Jomon, Extending the TraPPE Force Field for Organophosphorus Compounds: Triethyl Phosphate and Trimethyl Phosphate

New Jersey Institute of Technology
Authors: Geordy Jomon; Santiago A. Flores Roman; Andrei Kolesnikov; Gennady Y. Gor

Studying the physical properties of organophosphorus chemical warfare agents (CWAs) is challenging due to their extreme toxicity. To mitigate this risk, experimental studies use CWAs simulants – organophosphates with similar molecular structures and physical properties that are less toxic for their use in laboratories. These similarities to CWAs allow for the development of protective equipment and methods for detection and decontamination. Diisopropyl methylphosphonate (DIMP) is among the most used CWA simulants. However, the market accessibility of DIMP is limited, and therefore, its laboratory use is costly. Triethyl phosphate (TEP) emerges as a promising CWA simulant, offering higher market accessibility due to its numerous industrial applications. Molecular simulations can extend known literature data for numerous target fluids while utilizing force fields to model them accurately and realistically. Simulants, such as DMMP and DIMP, have been studied using this approach [1, 2]. Here, we model and characterize TEP based on the transferable potentials for phase equilibria (TraPPE). We use TraPPE descriptions of known organophosphates in the literature and transfer their atom, bond, angle, and dihedral interaction parameters to TEP [2]. Additionally, ab initio calculations were performed to obtain the remaining parameters – dihedral interactions using potential energy scans, and partial charges [3]. To validate the model, we performed molecular dynamics (MD) simulations to predict the liquid densities and compared our predictions with available literature data [2, 4, 5]. Furthermore, Gibbs ensemble Monte Carlo simulations were performed to model vapor-liquid phase behavior. From these simulations, we compared the simulated vapor pressures to experimental values and calculated their critical parameters [6, 7]. We also performed MD simulations to predict the enthalpy of vaporization, surface tension, viscosity, and diffusivity. Moreover, we also parameterized and characterized trimethyl phosphate (TMP) due to its structural similarity to TEP. Our study will help assess TEP and TMP as alternative simulants and provide predictions of their physical properties, i.e., liquid densities, vapor pressures, enthalpy of vaporization, surface tension, viscosity, and diffusivity, in a wide range of temperatures.

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2.8 Gizem Chelebi Torabfam, Toward Safer Melittin-Based Therapeutics: Tuning Pore Formation via Terminal Polarity

New Jersey Institute of Technology
Authors: Gizem Celebi Torabfam; Sandeepani Punyakanthi Thilakaratne; Cristiano L. Dias

Antimicrobial and anticancer peptides represent a promising class of therapeutics due to their ability to selectively disrupt microbial and cancer cell membranes. Melittin, a well-studied peptide from honeybee venom, exhibits potent lytic activity but suffers from severe cytotoxicity. In this study, we focus on a shortened melittin variant having 11 amino acid residues, which retains antimicrobial potency while displaying reduced cytotoxicity. Using molecular dynamics simulations, we provide computational insights into its mechanism of membrane disruption in mixed DMPC/DMPG bilayers. Our findings reveal that this variant rapidly induces toroidal pore formation,

facilitating translocation of water molecules across the bilayer. To further dissect the molecular determinants of pore formation, we engineered C-terminal mutations to compare apolar versus polar residues. Remarkably, peptides with apolar termini failed to form pores, whereas serine- and threonine-terminated peptides promoted efficient water translocation within only 2 microseconds. Moreover, polar-ended variants induced pronounced membrane thinning, in contrast to their apolar counterparts, highlighting the critical role of terminal polarity in modulating peptide–membrane interactions. Together, these results provide new mechanistic insight into the balance between peptide sequence, pore formation, and membrane perturbation. Our study suggests rational strategies for designing next-generation melittin-based therapeutics with enhanced selectivity and reduced cytotoxicity.

2.9 Haoxuan Li, Coarse Grained Molecular Dynamics Simulations of Organic Mixed Ionic-Electronic Conductors

Lehigh University
Authors: Haoxuan Li; Mitchell Hausback; Thomas E. Gartner III

Organic mixed ionic-electronic conductors (OMIECs) are soft materials that enable simultaneous transport of ions and electronic charge carriers, making them promising candidates for bioelectronics and organic electrochemical transistors (OECTs). Recent studies show that carboxyl-alkyl functionalized polythiophenes, such as poly[3-(4-carboxybutyl)thiophene-2,5-diyl] (P3CBT), exhibit low swelling and high OECT performance. Both cations and anions participate during electrochemical doping and de-doping processes in these systems, yet the molecular-level structure during device operation–and how microscale structure impacts electronic properties–remains poorly understood. To investigate these connections, we developed a coarse-grained molecular dynamics (CG-MD) model for P3CBT inspired by work by Savoie and coworkers on CG simulations of polythiophenes. We varied the backbone oxidation level and the protonation state of the carboxylic acid side chains to mimic experimental changes in ion concentration and pH. Our model allows us to characterize trends in the association between ions and polymer segments, which we use to rationalize prior experimental results on P3CBT. In ongoing work, we examine the effects of key design parameters such as ion identity, ion concentration, and polymer side chain chemistry on the molecular-level structure of OMIECs, ultimately providing insights to guide the development of next-generation bioelectronic materials.

2.10 Jianping Chen, Molecular Dynamics Simulations of Fibril Formation of Chiral Peptides

New Jersey Institute of Technology
Authors: Jianping Chen; Cristiano L. Dias

Two-dimensional infrared (2D IR) spectroscopy experiments have shown that peptide chirality strongly influences fibril formation. Specifically, the number of β-sheets differs when only left-handed peptides are present compared to when both left- and right-handed peptides are combined. Understanding how left- and right-handed peptides assemble—whether through self-assembly (homochiral), mixed assembly (heterochiral), or random association—remains an important open question. To address this, we performed molecular dynamics simulations on five different peptides. For each peptide, two simulations were carried out under identical conditions (350 K, 2 μs): one with ten left-handed peptides and another with a mixture of five left- and five right-handed peptides. From the simulations, we analyzed secondary structure evolution, Cα and residue arrangements, and hydrogen bond formation within and between homochiral and heterochiral peptide pairs. Additionally, we calculated van der Waals and Coulomb energy changes to evaluate energetic preferences. Together, these results provide molecular-level insight into the role of chirality in peptide fibril formation.

2.11 Mansi Gokani, Computational Evaluation of Polystyrene Binding Polypeptides

Rutgers New Brunswick
Authors: Mansi Gokani; Brianna Fea; Ashley Guo

Micro- and nanoplastic waste poses significant environmental and health concerns due to their increased likelihood of consumption as they break down from larger plastic waste. Freshwater is highly contaminated with these plastics, as current water filtration methods are ineffective at the nanoscale. To address this issue, new materials and methods are needed to capture and remove nanoplastics from water. Peptide based materials are ideal due to their ability to perform functions with highly specific molecular recognition. However, the vast design space of

amino acid sequences necessitates computational methods for screening and identifying peptide sequences capable of selective binding to target plastics. Furthermore, an evaluatory method is needed to determine if a given plastic binding peptide is effective for a target plastic. We approach these challenges by using molecular dynamics simulations with enhanced sampling methods to determine if a candidate peptide sequence can be used to capture nanoscale polystyrene. With the addition of free energy calculations and analysis of binding configurations, we present a thermodynamic understanding of successful polystyrene capture with solvation analysis that can inform optimized design of nanoplastic-sequestering materials.

2.12 Minh-The Hoang, Local Onsager Matrix in Confined Fluids

Princeton University
Authors: Minh-The Hoang; Ian C. Bourg

Understanding transport phenomena in confined fluids is a central challenge in modern liquid state theory. When liquids are restricted to nanometric dimensions—within porous media, mineral interfaces, or synthetic and biological nanopores—the surface-to-volume ratio increases dramatically, amplifying interfacial interactions and molecular-scale inhomogeneities. This geometric shift heightens sensitivity to local structure, dynamics, and external gradients, enabling precise control over coupled transport phenomena such as electro-osmosis, thermo-diffusion, and voltage gating. These mechanisms have driven significant technological advances across diverse applications, including energy harvesting/storage, water purification, and nanopore sequencing.

Although continuum descriptions of coupled transport perform well over a broad spectrum, thermal fluctuations, adsorption effects, electrical double layers, and molecular friction dominate behavior at the nanoscale and require atomistic considerations. To address this challenge, we introduce a unified methodology that leverages a space- and time-dependent response matrix to probe the intricate dynamics of confined fluids from molecular simulations.

Our study is based on a generalized linear response relation linking the local fluxes $j_a(\mathbf{r}, t)$ of fluid, solute, heat, and charge, and spatially and temporally varying conjugate driving potentials $\phi_b(\mathbf{r}', t')$ (pressure, chemical potential, temperature, and electric potential). The coupled linear response is encapsulated in a response kernel $K_{ab}(\mathbf{r}, t; \mathbf{r}', t')$ accounting for non-local and memory effects. We employ equilibrium molecular dynamics and an extended Green–Kubo formalism to extract this kernel from local fluctuations and connect microscopic interactions to collective transport in modeled confined fluids. Using this framework, we analyze fundamental processes—such as molecular layering, advection/diffusion of solutes and heat, and charge relaxation—and examine how coupled transport emerges across different temporal and spatial scales.

Beyond providing local transport properties, this method also serves as an explicit bridge to various established hydrodynamic theories such as dynamical density functional theory or mode coupling theory, thereby advancing the understanding of fluid transport at the nanoscale. The insights gained contribute to a deeper comprehension of solid-fluid interfaces, with significant implications for nanofluidics, electrochemistry, and various technological applications.

2.13 Noor Aldin Alzghoul, ML based computational prediction of catalytic nanoparticle shapes

Rowan University
Authors: Noor Aldin Alzghoul; Dr. Aditya Lele

The surface facets control surface catalytic activity. Precise prediction of surface energies is critical in determining surface catalytic interactions, which is a key consideration in chemical conversion using nanoscale catalysts. Density Functional Theory (DFT) calculations are the standard method to determine surface energies (SE). Their computational cost means that they are impractical for large material screening and simulations considering realistic conditions. Machine learning interatomic potentials (MLIPs) are an alternative approach that can potentially provide the computational speed and accuracy required to predict surface energies. However, existing MLIPs either need large amounts of DFT training data for accurate SE prediction or have relatively limited accuracy when trained as large-scale models. To address this limitation, we aim to utilize transfer learning techniques—starting with MLIPs trained on minimal or lower-accuracy data and progressively refining them with targeted, high-accuracy DFT surface datasets. Specifically, these ML potentials are improved step-by-step by integrating precise DFT calculations for common low Miller indices (100), (110), and (111) before expanding systematically to higher Miller indices. Then, to ensure that these refined potentials accurately capture real-world conditions, they are further optimized for finite-temperature environments, allowing them to better model realistic thermal surface behaviors. Additionally, we aim to evaluate different combinations of lower-accuracy and high-accuracy data to determine the

best balance between computational efficiency and predictive precision. This comprehensive approach enables fast and precise surface energy predictions at a significantly accelerated pace, facilitating the discovery and development of advanced materials.

2.14 Punyakanthi Sandeepani Thilakaratne, Adsorption of Amphipathic Peptides on Lipid Membranes: Effects of Lipid Headgroup Size and Acyl Tail Length

New Jersey Institute of Technology
Authors: Punyakanthi Sandeepani Thilakaratne; Jirasak Wong-Ekkabut; Cristiano L. Dias

Peptide-membrane interactions play a pivotal role in a range of biological processes including antimicrobial activity, drug delivery, and the formation of amyloid aggregates. Their selective binding behavior depends not only on peptide sequence but also on the physicochemical properties of the target membrane. Using all-atom molecular dynamics simulations, we systematically investigate the influence of lipid headgroup chemistry and acyl tail properties on the adsorption behavior of amphipathic model peptide Ac-AKFEFKAE-NH2. Here, fourteen model membranes comprising of PC:PG or PE:PG mixtures with varied tail lengths and saturation states were simulated. Our results show that membranes containing phosphatidylethanolamine (PE) headgroups consistently exhibit higher peptide adsorption than those with phosphatidylcholine (PC), primarily due to enhanced electrostatic interactions and greater accessibility of PG headgroups in the PE:PG mixture. Furthermore, unsaturated acyl tails, despite their longer length, facilitate stronger peptide binding compared to saturated ones, highlighting the dominant role of tail disorder over chain length. Peptides exhibit higher tilt angles and stronger binding in PE membranes, unlike PC systems which have less available space due to bulk headgroup size. These findings underscore the critical role of lipid headgroup identity and tail saturation in governing peptide-membrane interactions.

2.15 Quinn M. Gallagher, An Interpretable Machine Learning Tool for the Classification of Atomic States in Molecular Simulations

Princeton University
Authors: Quinn M. Gallagher; Ryan J. Szukalo; Nicholas Giovambattista; Pablo G. Debenedetti; Michael A. Webb

Molecular dynamics (MD) simulations are often used to analyze mixtures and transitions in materials at atomic resolution. However, it can be difficult to identify collective variables that describe the extent to which an atomic environment belongs to one state or another, hindering the ability of MD simulations to characterize mixtures and transitions. We present a data-driven approach to automatic collective variable identification, and we use this approach to analyze MD simulations of transitions between high-density amorphous (HDA) and low-density amorphous (LDA) ice. Specifically, we show that a minimally redundant and maximally informative set of atom-centered symmetry functions and bond-orientational order parameters can be used to classify HDA and LDA environments at accuracies comparable to deep learning methods. Additionally, by using this set of descriptors in a probabilistic model, our classifier can identify outlier structures (i.e., hexagonal ice) without additional training. Our model's simple formulation enables an interpretable understanding of differences between HDA and LDA structure, quantifies compositions of HDA and LDA in simulations of transitions between the two states, and can be used to compute thermodynamic properties associated with these transitions. Finally, we show that our model is capable of identifying structural differences between atomic environments generated by different models of water, highlighting our method's potential to evaluate the similarities and differences of different force fields. Overall, this work shows how applying machine learning to ensembles of local atomic environments from MD simulations can reveal interpretable insights into materials behavior and simulation model fidelity.

2.16 Santiago Flores Roman, In Silico Test of the Gassmann Theory in Fluid-Saturated Nanoporous Glass

New Jersey Institute of Technology
Authors: Santiago Flores Roman; Geordy Jomon; Gennady Gor

Mechanical properties of fluid-saturated materials commonly differ from their unsaturated phase due to molecular interactions between adsorbates and adsorbents. As an example, previous studies of CO2 adsorption in zeolite X, have shown that the isothermal bulk modulus of the CO2-zeolite composite, a property intrinsically related to the isothermal compressibility, is commonly enhanced compared to the modulus of the unsaturated zeolite [1]. A number of methods have been developed to predict or estimate the bulk modulus of solid-fluid composites. For

instance, the Gassmann theory, a theory commonly used in geoscience, has been developed to estimate the bulk modulus of a composite from its constituents – confined fluid, dried porous material, and non-porous material [2]. Although, initially, this theory was developed to estimate the elasticity of macroporous materials, previous studies have shown proof of its applicability in fluid-saturated nanopores. Gor and Gurevich estimated the bulk modulus of argon and n-hexane adsorbed in Vycor glass from the Gassmann theory and obtained qualitative matches with results in literature [3]. More recently, Ogbebor et al. used the same theory to estimate the elasticity of water adsorbed in Vycor glass [4]. However, in all cases, the elasticity of the non-porous constituent needs to be estimated from approximation theories, which brings poor accuracy when calculating the modulus of the solid-fluid composite. As a consequence, the applicability of the Gassmann theory in nanoporous materials has yet to be accurately proven. Molecular simulations can overcome this limitation through a more robust approach – the bulk moduli of a solid-fluid composite and its constituents are calculated separately. In this work, we modeled gallium introduced in silica using both Monte Carlo and molecular dynamics, to predict the gallium-silica's bulk modulus and its constituents – confined gallium, porous silica, and non-porous silica. Elastic deformations were used to predict the moduli of the composite, dry silica, and non-porous silica, while fluctuation theory was used to predict the modulus of confined gallium. Preliminary results show a decrease of the silica's bulk modulus as a function of the pore size, as well as a decrease of gallium's bulk modulus, even below the modulus of its bulk phase, caused by the solvophobicity of silica to gallium. The bulk modulus of the gallium-silica composite is yet to be predicted. This work aims to provide wider knowledge on the use of the Gassmann theory in nanoporous materials, and a deeper insight into the mechanical properties of fluids in solvophobic materials.

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