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Biophysical Modeling of the Active Transport of Actin Bundles in Plant Cells
Kwaku Acheampong, University of Tennessee,, Knoxville

In flowering plants, successful fertilization requires the migration of the sperm nucleus through the large, vacuolated central cell toward the female nucleus. This movement depends on the bulk motion of F-actin bundles, with molecular motors playing a key role in driving the transport. While actin-dependent nuclear movement has been reported in various plant systems, the mechanisms underlying sperm nuclear migration in the central cell remain unresolved. Recent experimental observations suggest that clustered, membrane-associated myosin motors bias the movement of F-actin bundles linked to the migrating sperm nucleus. To investigate the underlying biophysical mechanisms, we developed a computational model in Cytosim that simulates actin filaments that are bundled by crosslinking proteins and actively transported by myosin motors immobilized on a surface. Our simulations reveal that bundled filaments can exhibit persistent directional motion when interacting with spatially clustered motors. Filament movement depends sensitively on the degree of crosslinking and the geometry of motor clusters: moderate crosslinking promotes coordinated motion, while excessive crosslinking impedes mobility. Additionally, both the size and spatial distribution of motor clusters affect the persistence of filament movement. These results suggest that the organization of motors and bundling proteins may enable directed transport of actin filaments in the central cell. Our model provides a controlled framework for exploring how filament bundling and the spatial arrangement of membrane-anchored motors contribute to organelle positioning during plant fertilization.

Computational Discovery of Potential Green Refrigerants Using Molecular Modelling and Machine Learning Barnabas Agbodekhe, University of Notre Dame

The 2016 Kigali Amendment mandates the phaseout of hydrofluorocarbons (HFCs). HFCs are widely employed as refrigerants but contribute significantly to global warming. This phaseout requirement has created an urgent need for developing environmentally sustainable refrigerant alternatives which we call green refrigerants. Previous works in green refrigerant discovery have primarily relied on screening large databases of chemical compounds such as PubChem. These previous works suggest that pure component fluid options for green refrigerants do not exist. This work combines optimization based mathematical programming with open-source isomer-enumeration algorithms for near-exhaustive candidate molecule enumeration, thereby avoiding the need to rely on limited databases of compounds. Group contribution, and sigma profile based molecular modeling were used in conjunction with Gaussian process regression and other machine learning models for reliable thermophysical and thermochemical property predictions with uncertainty estimates. The predicted properties, including thermophysical, environmental, and safety properties were used in screening and identifying the most promising candidates. Furthermore, this work demonstrates that current chemical databases do not exhaustively cover the chemical design space even for very small molecules like refrigerants.

Mechanisms of daptomycin insertion into bacterial membranes: Insights from molecular dynamics simulations Ali Al-Najada, University of Tennessee, Knoxville

Enterococcus faecium is a Gram-positive bacterium known to cause various infections. Daptomycin is a cyclic lipopeptide that has been used clinically to treat Gram-positive bacterial infections including E. faecium infection. Its suggested mechanism of antibacterial action involves insertion into the bacterial membrane in a manner that depends on calcium and the phosphatidylglycerol (PG) content of the membrane. However, studies have focused primarily on interactions of daptomycin with simple model membranes, and there is limited understanding of its interactions with more complex and realistic membrane compositions. In this study, we used all-atom molecular dynamics simulations to investigate daptomycin's insertion into realistic membranes. We used experimentally-determined membrane compositions for clinically-isolated strains of E. faecium (TX0016 and TX1300) in two different growth conditions (BHI and serum). Simulating the membranes in the presence of calcium, we characterized daptomycin's tail insertion into the membranes in terms of the equilibrium depth of insertion and the potential of mean force as a function of the insertion depth. We also investigated the contact of daptomycin residues with various lipid headgroups, the formation of salt bridges between daptomycin and lipids, and the impact of daptomycin on properties of the membranes. When multiple daptomycin molecules were present, we found that they interacted with each other both before and after insertion into the membrane. This work improves our understanding of daptomycin's insertion into bacterial membranes and its impact on the membrane properties, which may help to explain differences in its efficacy for bacteria grown in different conditions.

Computational Mechanochemistry Alex Albaugh, Wayne State University

Mechanical forces can break chemical bonds, and chemical reactions can generate mechanical forces. Here we will share simulation and theoretical studies exploring both paradigms. We will present the rheological properties of mechanically interlocked polymers in flow. These polymers, characterized by topological links akin to chains, display unique flow behaviors, including lower stresses and increased tumbling compared to linear polymers. Our simulations reveal that fluid-induced mechanical forces can cause both chemical degradation through bond cleavage and physical degradation through slippage of interlocked components. Additionally, we will present our recently developed model for myosin, a biological molecular motor. This motor has two heads that walk hand over hand along an actin track. This motion generates mechanical forces from the hydrolysis of adenosine triphosphate (ATP). The model captures the full chemically driven cycle of myosin walking and opens the door to detailed thermodynamic study of its entropy production, efficiency, and mechanism. Taken together, our results showcase the interconnected roles of mechanical forces and chemical reactions in complex molecular systems.

ChIMES Machine-Learned Interatomic Models for in silico Design of Zeolite Membranes Sayed Ahmad Almohri, University of Michigan - Ann Arbor

Zeolite nanosheet membranes hold promise for transforming ammonia synthesis by integrating catalysis and separation into a single unit operation, yet optimizing their design requires atomic-scale insights into reactive interfaces that govern stacking motifs and dynamics. Traditional simulations face a fundamental trade-off: quantum mechanical methods like density functional theory (DFT) are computationally prohibitive for large systems, while classical force fields lack the accuracy to describe reactive events critical to nanosheet interactions. To bridge this capability gap, we develop a machine-learned interatomic model (ML-IAM) for simulating zeolite materials relevant to ammonia synthesis using the Chebyshev Interaction Model for Efficient Simulations (ChIMES) framework. ChIMES is a unique physics informed ML-IAM and semi-automated fitting framework that combines the accuracy of DFT with the computational efficiency of molecular mechanics, which has been successfully applied to study the behavior of multiple chemical systems. Here, we discuss application of ChIMES to characterization and optimization of MFI-type zeolite nanosheet membranes. The model is first parametrized for Si-O interactions in bulk zeolites, validated against DFT data to ensure fidelity to quantum-mechanical behavior. We then extend ChIMES to capture interfacial interactions in hydroxylated nanosheets, addressing the complex bonding dynamics critical to membrane assembly. Molecular dynamics simulations reveal how nanosheet alignment and stacking motifs influence pore structure, guiding design strategies for enhanced selectivity. By resolving atomic-scale reactivity and mesoscale membrane morphology, we establish ChIMES as a transformative tool for in silico screening of zeolite membranes, advancing computational capabilities for energy-efficient catalytic reactors.

Effect of polyelectrolyte degree of polymerization on coacervate structure and phase behavior Kayley Alonso, University of Notre Dame

Complex coacervation, a liquid-liquid phase separation phenomenon, occurs when oppositely charged colloidal species form a dense phase through electrostatic interactions. This process drives the formation of polyelectrolyte complexes (PECs), which are of considerable interest across diverse fields, including biotechnology, pharmacy, medicine, and material science. The structure, dynamics, and thermodynamic properties of PECs are known to be influenced by factors such as the topology, size, and charge density of the constituent polyelectrolytes. Due to their versatility, tunability, and biocompatibility, PECs have garnered considerable scientific interest. However, molecular dynamics (MD) simulations of complex coacervation have been limited: existing simulations involve implicit solvent and fail to capture relevant entropic effects. Furthermore, implicit solvent simulations provide less detailed insights into the internal structure of the dense coacervate phase.

In this work, we focus on how the degree of polymerization (N) of polyelectrolytes influences these metrics crucial for PEC tunability. By employing a model that incorporates explicit solvent molecules and polyion beads, our simulations reveal that the stability of the coacervate phase increases with N. Additionally, we observe that polyelectrolyte chains within the coacervate adopt conformations consistent with good solvent conditions, exhibiting a Flory exponent with weak temperature dependence. Furthermore, the compactness of the coacervate is found to be largely independent of chain length. These findings are consistent with prior theoretical predictions and experimental observations and provide a solid basis on which to build new insights on the energy–entropy interplay within PECs.

Binder Desorption Mechanisms from Polyethylene Films via Molecular Dynamics of Surfactant-Mediated De-inking Ali Altamimi, University of Wisconsin-Madison

Printed inks are a common contaminant in plastic packaging and are known to degrade the color or transparency, mechanical properties, and odor profile of mechanically recycled plastic films. Polymeric binders, typically ranging from 10,000 to 30,000 g/mol, constitute the majority of the ink mass after drying. A proven method for ink removal involves pre-treating the feedstock by rinsing it in a cetrimonium bromide (CTAB) or other surfactant solution above the critical micelle concentration (CMC) under basic conditions (pH 11–13) for 1–3 hours with agitation.To elucidate the mechanism of de-inking, both all-atom and coarse-grained molecular dynamics (MD) simulations were performed. The solubilization of two common binders—polyether urethane (PEU) and nitrocellulose (NC)—was evaluated in a range of cationic, anionic, and nonionic/amphoteric surfactants. Nonionic surfactants exhibited the highest solubilization of PEU and NC, likely due to the absence of electrostatic repulsion between surfactant headgroups. Additionally, adsorption and desorption free energies of the binders from a polyethylene (PE) thin film were computed in water and in the presence of surfactants at different concentrations using umbrella sampling. At high charged surfactant concentrations, binder desorption free energies decreased from approximately 450 kJ/mol in water to 350 kJ/mol or lower.

Entropy and Bias based Decision Lattice - A theoretical characterization of Cognitive Path Dynamics using tools from Statistical Physics and Thermodynamics Subhangshu Sen and Yashdi Saif Autul, Rensselaer Polytechnic Institute

Our work presents a fully analytical framework to model cognitive decision-making as structured information trajectories on a decision lattice, using tools inspired by statistical physics, field theory and thermodynamics. Each node in the lattice represents a decision point and is classified as either bosonic (multi-outcome, entropy-generating) or fermionic (binary yes-no, bias-amplifying). By assigning probabilistic weights to each outcome, we define two key constructs: the Decision Entropy Functional - quantifying cognitive flexibility and the Bias Accumulation Functional - capturing the structural and probabilistic rigidity of the decision path. Reinforcement-conditioned memory is introduced through geometric weights, enabling us to analyze how past memory or reinforced learning slows down entropy decay and saturates the rate of bias accumulation, by introducing a soft ceiling. We show analytically that while entropy typically decays with increasing node depth, bias tends to accumulate — eventually leading to a loss of free will situation. Our model identifies the analytical threshold at which a sufficient number of fermionic nodes (irrespective of the number of intervening bosonic nodes) causes decision crystallization, thereby collapsing the path into a structurally rigid regime.

To reverse this, we introduce the idea of bosonic re-injection, whereby high-entropy bosonic nodes act as “quantum tunnelers” or entropy gateways and induce a phase transition that reopens the decision landscape. We derive thresholds for the number and entropy contribution of bosonic nodes required for this de-crystallization. Moreover, we establish a mathematical criterion for a glass transition - where though configurational entropy of the choice space remains high, but is severely suppressed by memory-based bias — thereby creating a kinetic barrier that renders these choices inaccessible and leads to a state of decision paralysis. Our theory unifies the concepts of free will, information theory and decision dynamics into a coherent, novel formalism. It provides a new foundation for modeling cognitive rigidity, adaptive recovery and bounded rationality. Applications span across diverse domains - including behavioral economics (e.g., market inertia and policy reversibility), moral psychology (e.g., ethical gridlocks and resolution dynamics), AI decision frameworks (e.g., entropy-aware planning in constrained environments) and niche applications in clinical neuroscience (e.g., modeling cognitive freezing in anxiety or executive dysfunction). By identifying when and how decisions crystallize, liquify or become glass-trapped - our theory offers both analytical insight and actionable implications for cognition-driven systems.

Machine Learning Force Fields for Ion Hydration: Evaluating MACE Foundation Models for Alkali and Alkaline Earth Ions Zachary Baker, University of Kentucky

Machine learning (ML) force fields have emerged as powerful tools for molecular simulations, offering accuracy comparable to ab initio methods while maintaining the efficiency required for large-scale simulations. These models learn interatomic interactions from quantum mechanical calculations, enabling a more transferable and data-driven approach to force field development. Among ML-based approaches, MACE (Message-Passing Atomic Cluster Expansion) foundation models represent a significant advancement, leveraging equivariant neural networks to capture complex many-body interactions.

In this study, we assess the ability of MACE foundation models to describe the hydration behavior of common ions—Li^+, Na^+, K^+, Mg^{2+}, and Ca^{2+}—in aqueous environments. We compare MACE-based simulations with conventional empirical force fields and reference ab initio molecular dynamics data, evaluating structural and dynamical properties such as radial distribution functions, coordination numbers, self-diffusion coefficients, and hydrogen bond lifetimes. While ML force fields offer improved accuracy in capturing short-range quantum interactions and electronic polarization effects, challenges remain in data efficiency, transferability to diverse chemical environments, and computational cost. Our findings highlight the strengths and limitations of MACE models in ion hydration studies and their potential to bridge the gap between empirical and ab initio methods in molecular dynamics simulations.

Molecular Level Understanding of Thermodynamics of Complexation for Selective Separation of Lanthanide Ions in Aqueous Solution Sayani Biswas, The Ohio State University

Lanthanides are a subset of rare earth elements (REEs) that are essential components in smart phones, electric vehicles and wind turbines. Current REE recovery processes are resource intensive and produce hazardous wastes. Developing a sustainable REE recovery process requires new techniques that are economical and less wasteful, such as selective separations from wastes. Enabling selective separation techniques require ligands, such as peptides, that bind strongly to lanthanides and exhibit selectivity towards individual lanthanides in aqueous environments. Peptides are short chains of amino acids that are tunable, i.e., their properties can be modified by changing the constituent amino acids, making them a suitable choice for ligand design. Particularly, the lanthanide binding peptide EF handloop 1 of Lanmodulin (LanM 1) is chosen as the initial ligand design for separations because it selectively binds to lanthanides over other metal ions to form complexes. In this work, we use classical molecular dynamics (MD) to estimate the free energy change of aqueous complexation of LanM1 peptide, and its design variants, with the REEs Lanthanum (La3+), Cerium (Ce3+), Praseodymium (Pr3+), and Neodymium (Nd3+). We extract the entropic and enthalpic components of the complexation reaction and show that the entropic component drives the overall reaction while the enthalpic component of free energy of complexation is negligible. We investigate the influence of different descriptors on the complexation reaction, such as, change in radius of gyration of the peptide and water rearrangement in the first solvation shell around lanthanides. These insights can then be used to learn how ligand design can be tuned to enable selective REE separations.

Coarse-Grained Modeling of Polymer-Grafted Nanoparticle Monolayers with an Adjusted Angle Potential Jacob Breese, The Ohio State University

Polymer-grafted nanoparticle (PGN) monolayers offer significant advantages over traditional homopolymer or bare nanoparticle composite systems by leveraging self-assembly to form mechanically robust, highly ordered materials. The structural and mechanical properties of these monolayers are influenced by adjustable PGN characteristics, including polymer chain length and grafting density. We employ a coarse-grained simulation approach incorporating a colloidal potential to model nanoparticle interactions and an angle potential adjusted to map the Kuhn length and density to a specific polymer type. We examine several PGN systems, both above and below the entanglement length. Following equilibration, radial distribution functions and density profiles are analyzed to understand differences in nanoparticle and monomer packing. As expected, above the entanglement length, lower graft density increases interpenetration and interparticle double kinks per chain. Systems with varying graft densities and chain lengths but similar polymer content exhibit similar nanoparticle spacing. The addition of a stiff angle potential increases entanglements per chain in comparison to a freely rotating model used in prior work.This research was supported in part by the Air Force Office of Scientific Research under GR131498.

Modeling the non-Brownian motion of non-enveloped reoviruses on membrane surfaces
Greg Cantrall, University of Tennessee,, Knoxville

Non-enveloped viruses lack a surrounding membrane, yet they must engage with and breach host cell membranes as a key step in the infection process. Recent studies of the non-enveloped reovirus have demonstrated that infectious subvirion particles (ISVPs) adhere to lipid membranes and undergo non-Brownian motion. The mechanisms behind the non-Brownian movements are currently unknown, but it is hypothesized that peptides on the surface of the ISVP play a role. These peptides insert into the membrane, are cleaved, and then diffuse and aggregate in the membrane. To investigate biophysical mechanisms underlying ISVP motion, we developed a stochastic computational model of ISVP motion and used the Gillespie algorithm to generate stochastic trajectories describing the motion of ISVPs and cleaved peptides. In the model, insertion of a peptide on the capsid generates directed motion on timescales associated with peptide cleavage. Once cleaved and part of the membrane, peptides can locally trap an ISVP due to their mutual attraction. We assessed ISVP motion by characterizing the mean square displacement (MSD) and distribution of angles between segments of its random motion. The ISVPs exhibit directional motion at short times that transitions to locally confined motion at long times. Further, faster peptide cleavage promotes the formation of larger peptide clusters because peptides are cleaved in closer proximity and can more readily aggregate. The simulation results suggest that the motion of individual ISVPs can be segmented into various types of motion, with large, directed excursions interspersed with confined motion induced by relatively immobile peptide clusters.

Impact of gas phase loading, dipole moment, and configurational variability on the optical response of JETVOW for optical sensing Ricardo A. Garcia Carcamo, University of Notre Dame

Quantum sensing is an emerging technology with promising future applications. Among various of these techniques, optical sensing offers a non-invasive and potentially selective method for detecting optically active molecules. Non-centrosymmetric porous materials that exhibit Second Harmonic Generation (SHG) are promising candidates for such sensors. In this study, we investigate the effects of molecular loading and configurational variability of gas-phase molecules with different dipole moments on the optical response of JETVOW, a relatively large non-centrosymmetric porous material. We hypothesize that molecules with higher dipole moments and greater loadings induce larger changes in the material's optical response. To test this hypothesis, we employ a combination of classical Monte Carlo simulations to generate different configurations of gas-phase molecules and quantum mechanical calculations to determine their optical properties and ultimately estimate the ensemble average for a given loading. Our results indicate that the optical response depends on the type of molecule, the loading, and the spatial orientation of the gas-phase molecules.

The Effects of Temperature and Adsorption on Free Energy Profiles of Soft Porous Coordination Polymers James Carpenter, University of Notre Dame

Soft porous coordination polymers (SPCPs) are flexible porous materials comprised of metal-organic polyhedrons (MOPs) connected by organic linkers, with potential in adsorption applications. Various SPCPs have been shown to exhibit novel and/or useful adsorption properties such as negative gas adsorption (NGA), high deliverable capacity, and stimulus-responsive behavior which can be leveraged for such applications as gas storage, separations, and sensing. We performed molecular simulations of various SPCPs that vary in the length and flexibility of the organic linkers to address how the flexibility can result in various configurations and affects configuration stability. We examined free energy profiles as a function of volume of different SPCPs while varying both methane loading and temperature, resulting in different stable configurations of interest. We found significant differences in the volume of the stable phases and the number of phases present, with more flexible linkers having more stable configurations. We also characterized the textural properties of the various stable configurations for the SPCPs and analyzed density profiles of the methane in various configurations. Altogether, our examination can be used to understand the relevant configurations of the SPCPs at a given loading and temperature and provides molecular-level understanding of how the flexibility of the organic linkers affects the structure of the system at varying conditions.

Statistical Mechanical Insights into the Latent Space of Glasses Charles Carroll, University of Wisconsin-Madison

Despite their useful properties, the purposeful design of amorphous materials is limited by the lack of physical connection between atomic level structures and macroscopic observables. Molecular dynamics is a key tool in probing microscopic behavior in these materials. However, the raw data from these simulations is difficult to relate to meaningful physical insights. Traditional order parameters are usually designed to quantify specific kinds of structures, often corresponding to regular crystal structures. To characterize these more complex structures, we can borrow technologies from the machine-learned potential community, whose numerical descriptors are sensitive enough to delineate very similar configurations of particles. This work uses one such descriptor, the Smooth Overlap of Atomic Positions (SOAP), to quantify local chemical structures. We demonstrate this approach by using a transition-state framework to analyze the evolution of this distribution for a model glass forming potential, the Kob Andersen potential. We seek to identify the key event that enables crystallization at certain compositions and how other compositions resist crystallization into the thermodynamic minimum. We aim to maximize interpretability by using linear transformations and existing statistical mechanical methods.

Thermodynamic Stability of Chalcogenide Perovskites from First Principles Adelina Carr, University of Minnesota

Chalcogenide perovskites are emerging as promising candidates for optoelectronic applications due to their favorable bandgaps, high absorption coefficients, and tolerance to defects. Compared to oxides, they offer improved spectral match for solar harvesting; compared to hybrid halides, they exhibit better environmental stability. However, unlike their oxide counterparts, chalcogenide perovskites often suffer from thermodynamic instability due to polymorphic competition and phase decomposition.

In this work, Density Functional Theory was used to assess the thermodynamic stability of 81 ternary chalcogenides with the formula ABX_3 (A = divalent, B = tetravalent, X = S). Decomposition energies relative to known competing phases were computed to identify trends in phase stability. Additionally, we analyzed polymorph energetics to understand preferences for particular octahedral motifs (e.g., edge- or face-sharing). Comparison with tolerance factor predictions reveals that geometric criteria alone are insufficient to capture stability in these systems, highlighting the importance of thermodynamic analysis. By analyzing the electronic structure of materials in perovskite and non-perovskite structures, we relate the calculated thermodynamics to chemical bonding in these materials. This work shows how increased covalency in sulfides influences phase behavior in chalcogenide perovskites, shedding light on the origins of their structural and compositional instabilities.

Modeling hydrophobicity and charge fraction effects in complex coacervates using the transfer matrix method Jacob Castañeda, University of Illinois Urbana-Champaign

Complex coacervation is a phenomenon that occurs when charged polyelectrolytes are mixed within an aqueous solution and undergo phase separation into a polymer-rich coacervate phase and a polymer-poor supernatant phase. The physics of complex coacervation is relevant to relevant to many fields, such as cellular biology personal care products, and drug delivery; however, there is a vast parameter space that affects phase behavior such as salt concentration, charge fraction, hydrophobicity, stoichiometry, etc.

Our research is focused on the modeling of how charge fraction and hydrophobicity affect coacervation. Inspired by recent experiments performed by a collaborator (Prof. Laaser), we seek to understand the relationship between electrostatic and solvent-driven phase behavior as a function of charge stoichiometry. Her work demonstrates that these parameters significantly affect salt resistance, which quantifies the amount of added salt needed to observe single-phase behavior.

Our model will be described using a transfer matrix method developed by the Sing Group, which exploits an adsorption formalism that simplifies the three-dimensional polymer solution structure to a one-dimensional representation that can predict the effect of electrostatic interactions with a straightforward numerical calculation. This can be incorporated into an overall free energy description of the system, which is used to map the phase diagram of polymers with a variety of charge and hydrophobic fractions and can be compared against experimental data from our collaborators.

Classical Molecular Dynamics Simulations to Understand the Formation of Polymer-Amino Acid Assemblies Srija Chakraborty, University of Wisconsin-Madison

Amino acids, fundamental to living organisms, link biological processes with chemistry and materials science. Despite their simple chemistry, their diverse structures and functionalities enable the formation of biocrystals and complexes with remarkable properties, making them valuable for green and electronic applications. Recently, a breakthrough experimental study showed that hydroxyl-rich polyvinyl alcohol (PVA)-water interfaces can guide the formation of γ-glycine biocrystals. The γ-glycine polymorph is thermodynamically more stable but kinetically less favorable than the predominant α-glycine polymorph observed during homogeneous nucleation. Developing scalable production methods for γ-glycine biocrystals would be valuable for biomedical, semiconductor, and energy applications due to their exceptional piezoelectric properties, but the mechanism by which PVA promotes γ-glycine formation remains unknown, hindering further process development. The focus of the study is to look at different polymers and planar self-assembled monolayers (SAMs) to understand interactions between different functional groups with glycine and how these interactions impact glycine nucleation and polymorph selection. Using classical molecular dynamics (MD) simulations, we investigated the orientations and interactions between glycine molecules and SAM surfaces in the different systems to relate these to structural observables for known polymorphs. Three order parameters were used for comparison: the angle of glycine molecules with the normal to the SAM surface, the intermolecular angles of glycine molecules and the number of closed contacts between the glycine molecules and the SAM surface. The order parameters were used to compare six systems of aqueous glycine and SAMs with different functional groups at different pH values. These results are then compared with a system of crystallized γ-glycine to find the best conditions that promote the nucleation of γ-glycine. We find that systems representing polymer templates in low and isoelectric pH ranges lead to order parameters consistent with those found for γ-glycine polymorphs. Understanding the underlying mechanisms governing the heterogeneous nucleation of glycine and the role of interactions at the surface in promoting polymorph selection could help identify the most suitable polymer template to produce γ-glycine at a scalable level, and moreover generalizable design guidelines to promote the nucleation of amino-acid biocrystals.

Modeling the Morphology of Polymorphic Manganese Sulfide Nanocrystals Junchi Chen, Washington University in St. Louis

Many physical and chemical properties of nanocrystals—such as their preferred directions of crystal growth, the reactivity of their surfaces, and their ability to absorb different wavelengths of the electromagnetic spectrum—are closely tied to their geometries. At thermodynamic equilibrium, the morphology of nanocrystals can be approximated by applying the Gibbs-Wulff theorem, which directs the construction of the so-called "Wulff shape," whose surfaces minimize the total surface energy at constant volume. Although the equilibrium morphology of elemental systems is widely understood recently, that of binary compounds remains less explored.

In this talk, I will describe our analysis of the Wulff shapes of three experimentally synthesizable polymorphs of manganese sulfide (MnS) in a vacuum. We used density functional theory (DFT) to calculate the surface energy of various facets ranging from low to high Miller indices (up to 3). First, I will show that the r2SCAN exchange-correlation functional without van der Waals correction accurately reproduces experimental lattice constants and standard enthalpies of several materials and reactions relevant to synthesizing MnS. Second, when considering only the low-index facets, I will show that the Wulff shape of rock salt (RS-) MnS nanocrystals is cubic in sulfur-poor environments and octahedral in sulfur-rich environments. Our calculations predict polyhedra that are consistent with experimental observations and indicate that RS-MnS nano-cubes have facet-specific magnetic structures, where the (010) surface is ferromagnetic, while the (100) and (001) surfaces are antiferromagnetic. Third, based on the combination of slab and wedge models, I will show that the surface energies of polar facets in zinc blende (ZB-) MnS can be precisely separated, and the relative surface energy of polar facets in wurtzite (WZ-) MnS can be attained. Through this method, the asymmetric Wulff shapes of ZB- and WZ-MnS nanocrystals can be analyzed.

Crystallization Behavior of Crosslinked Polymer Networks Liang-Ching Chen, University of Illinois Urbana-Champaign

This study explores the crystallization behavior of crosslinked polymer networks using coarse-grained molecular dynamics simulations using HOOMD-blue. Building on the Kremer-Grest bead-spring model, we implement two distinct crosslinking approaches for comparison. In the first, monodisperse polymer chains are randomly crosslinked into a network before undergoing crystallization. While this method lacks specificity and does not replicate any specific chemical crosslinking process, it allows the investigation of general trends in how crosslinks affectcrystallization. In the second approach, crosslinks are introduced dynamically during polymerization using thiol-ene chemistry, enabling a more realistic formation of the network. We analyze the impact of these crosslinking strategies on crystallization by examining the overall degree of crystallinity, crystal domains, size and structure of crystal nuclei and precursors, and location of crosslinkers. These insights contribute to a broader understanding of polymer crystallization in constrained environments like networks and can inform the design of polymeric materials with tailored mechanical and thermal properties.

Mean-field phase behavior of binary vitrimer networks Yun-Ju Chen, University of Illinois Urbana-Champaign

Vitrimers, polymer networks featuring dynamic associative bonds, have garnered significant attention for their diverse applications, including self-healing, shape memory, and reprocessibility. The incorporation of phase-separating components in vitrimers further expands the design space for these properties. This study investigates the phase behavior of vitrimers formed by crosslinking binary blends with three-armed crosslinkers. We employ self-consistent field theory to model the phase behavior of these systems within the auxiliary field framework, innovatively avoiding explicit enumeration of products resulting from bond exchange reactions in the network. Instead of resolving explicit network topologies, we treat junction points as constraints in a mean-field fashion. This approach considers both the combinatorial entropy arising from the fact that junctions can be created by connecting polymer chains of different species, and the many possible arrangements of the chains between junctions. By doing so, we account for chemical differences stemming from the network's dynamic nature while quantifying the associated combinatorial entropy for the junctions. This research aims to provide deeper insights into the complex interplay between network dynamics and phase separation in vitrimers. By understanding these interactions, we can offer theoretical foundations for designing next-generation materials with precisely tuned microstructures, leveraging the unique properties of vitrimers to create innovative solutions.

Characterizing Pre-Gelation Recovery Rheology in Crosslinked Systems Benjamin Chiu, University of Illinois Urbana-Champaign

Strain sweep experiments for typical shear thinning viscoelastic materials observe a steady decrease of both the loss modulus (G") and the storage modulus (G'), with a crossover leading to a higher G", resulting in the material flowing. However, yield stress viscoelastic fluids will often observe an increase in G" as the material yields, then followed by the expected decline in G". This overshoot is theorized to be caused by the material's microstructure, which is then destroyed past a critical yield strain. Recent work by the Rogers Group has developed a constitutive model to describe this overshoot by breaking the G" into a recoverable, solid-like component, and an unrecoverable, fluid-like component. They attribute the overshoot due to a spike in the fluid-like G" as the material yields and begins to flow. This implies a continuous transition in yielding, rather than a single yield point.

During different time points during gelation, the viscoelastic material can exhibit different regimes of stress responses. At low extents of reaction, pre-percolated clusters in solution behave like shear thinning viscoelastic fluids. However, as the gel approaches the gel point, it begins to exhibit a yield stress fluid. As the fluid percolates during gelation, networks of crosslinked polymers are formed, creating more elastic, solid-like structures. However, how these percolating clusters result in varying stress responses is not well understood. To gain molecular-level insight of the material rheology during gelation, we will model the per-percolated network at varying extents of reaction. With cluster size distributions, we can characterize the recoverable and unrecoverable stress response of the system. With this we will show qualitative agreement in experimental rheological responses. In particular, we will focus on comparing the fluid-like and solid-like components of G" with the system confirmations to develop structure-property relationships for the stress response of percolating gels.

Topological Representations and Analysis of Binary Lennard-Jones Mixtures
Ethan Deutsch, University of Wisconsin-Madison

Topological Data Analysis (TDA) aims to represent and quantify the shape of complex datasets and with the goal of extracting useful information that can help characterize emergent phenomena. In the context of molecular dynamics simulations, this topological lens has been used to quantify the structure of gels and hydrogen bond networks to establish useful links between microstructure and emergent properties. However, the application of TDA to complex, multicomponent molecular systems is still underexplored. One such complex system is the Kob-Andersen (KA) binary Lennard-Jones mixture, a toy-system that is used for understanding glassy dynamics and crystallization. We hypothesize that the medium-range topology of the KA system can be used to better characterize its non-equilibrium phase behavior and understand what interactions lead to or hinder its crystallization. Using this model system, we derive topological representations of the binary systems and use this to characterize topological phase transitions. Our aim is to generalize these findings from the KA system to other binary mixtures and pave the way to deriving unifying topological representations for general multicomponent systems.

Development of Machine-learned Interatomic Potentials for coarse-grained simulation of molecular crystals Pratyush Dhal, University of Michigan - Ann Arbor

Atomistic or all-atom (AA) simulations are generally unable to reach the time scales necessary to capture nucleation or growth of molecular crystals. This problem is exacerbated for drugs, or active pharmaceutical ingredients (APIs) because their large size and complex structure further slows relaxation dynamics, requiring simulations on μs timescales. Coarse graining (CG) can possibly overcome this issue, mapping several atoms to a single interaction site, drastically reducing computational expense, but unfortunately, at the cost of reduction of accuracy. For example, recent work has shown that the well-known MARTINI

CG FF is not well-suited for modeling crystallization of even simple molecules. Lately, however, the use of machine learning to improve existing simulation models is becoming widely popular. Therefore, the goal of this work is to develop a strategy for using the ChIMES (the Chebyshev Interaction Model for Efficient Simulation) machine learned - interatomic model (ML-IAM) to bridge the accuracy gap between CG and AA simulations. The use of ChIMES ML-IAM should enable access to longer times and predict crystal growth in API with reasonable accuracy. The first step of this process involves establishing a reasonable CG model of simple molecular crystal followed by an assessment of the feasibility of the ML-IAM which is the primary focus of the work. In this work, we demonstrate how a ChIMES-generated CG FF for a simple organic molecular crystal, naphthalene, performs better than an existing MARTINI CG model for capturing the correct crystal structure

Uncovering Hydrophilic Protein Regions to Inform Nonfouling Surface Design
Lilia Escobedo, University of Pennsylvania

Biofouling, the contamination of surfaces with adsorbed biomolecules is a widespread issue that has significant repercussions on the longevity and effectiveness of equipment operating in aqueous environments. One strategy to address this issue is to coat surfaces with chemical groups that increase their wettability, promoting a hydration layer that prevents biomolecular adsorption. While polar and charged chemical groups are known to reduce surface biofouling, homogeneous coatings of these groups can be outperformed in nonfouling ability in real-world environments by coatings that incorporate chemical and charge heterogeneity, suggesting that heterogeneity can enhance surface hydration. To better understand this phenomenon, we seek inspiration from proteins, which have evolved heterogeneous surfaces to resist non-specific aggregation and fouling by other proteins in the crowded cellular environment. Additionally, since nanoscale heterogeneity has been shown to influence surface-water interactions in a non-additive manner, we do not use traditional additive measures of protein hydrophilicity, which sum individual amino acid contributions. Instead, we use specialized enhanced sampling molecular dynamics simulations that assess protein surface hydrophilicity directly based on how tightly individual protein surface atoms hold on to water. With this non-additive measure of hydrophilicity, we determine that hydrophilic protein surface regions contain similar fractions of polar and charged atoms as hydrophobic regions do, demonstrating that polarity alone is insufficient to determine protein hydrophilicity. We find that only charged groups are predominantly found in hydrophilic protein surface regions and that proximity to charged groups is a robust predictor of protein surface hydrophilicity. These results suggest that charged moieties behave like hydrophilic centers that influence the hydrophilicity of surrounding atoms and demonstrate that the chemical context of an atom's surrounding neighbors plays an important role in its hydrophilicity. Additionally, we observe that hydrophilic protein surface regions contain around 8.5% charged groups that have an approximate 1:1 charge ratio and are spread apart, and the remaining nonpolar and polar atoms are present in equal proportion. We believe that these characteristics of hydrophilic protein surface regions could be used to inform non-fouling surface design.

Structure-Property Relationships for the Thermophysical Properties of Ionic Liquids under External Electric Fields Fernando Javier Carmona Esteva, University of Notre Dame

New advancements in chemical separation processes are necessary to sustainably meet the increasing demand for electronics. Particularly, progress is needed in solvent design under the influence of external stimuli. Ionic liquids (ILs) offer an opportunity to investigate the effect of external stimuli such as external electric fields (EEFs) on separation media. ILs have thermophysical properties that make them attractive solvents for sustainable separation processes such as low volatility, high thermal stability, and tuneability of their thermophysical properties. Moreover, their charged nature makes them a great test case to investigate how the direct effects of EEFs on nanoscale dynamics and structure can impact the thermophysical properties of solvents under external stimuli. We uncover structure-property relationships for the thermophysical properties of ILs under EEFs by exploring the effects of external stimuli on structure, dynamics, and thermophysical properties through molecular dynamics simulations. For effects on structure, we quantify the effect of EEFs on nanoscale organization through excess entropy and its immediate consequences to dynamics by testing scaling relationships between self-diffusion coefficients and excess entropy under EEFs. Through excess entropy relationships, we are able to describe the entire dynamical landscape of a mixture and correlate systems that showcase distinct reactions to dynamics under external stimuli. With this understanding of dynamics, we also elucidate the emergent electrothermic properties of charged solvents in the presence of EEFs such as the electrostrictive and electrocaloric coefficients. Finally, with the implementation of novel methodologies to detect glass transition temperature from MD simulations, we explore the emergent phase-changing effect of EEF on ILs by correlating changes in excess entropy in the liquid phase to changes to the glass transition temperature. Such analysis allows us to establish connections between the glass and liquid phases and showcases how MD simulations can be leveraged to investigate the emergent behavior of ILs under EEFs, gain insights on the effects of EEF on the structural organization, and establish a better understanding of their thermophysical properties. With this insight we construct structure-property relationships for transport and thermophysical properties of IL in the presence of an EEF. Unlocking the control of transport and thermophysical properties through the manipulation of IL structure and EEF and eventually allowing for the next paradigm of separation schemes.

Free Energy Calculations of Host-Glucose Systems Mohsen Farshad, University of Notre Dame

Actively controlling blood sugar without using an external agent has yet to come to fruition. The glucose-responsive methods are paving the way toward developing an intelligent method to automatically control the glucose level. The glucose-responsive approach maintains glucose within a narrow physiological range to avoid high or low blood sugars. Here, we search for macrocycles that potentially can incorporate into this approach. To this end, we first study the glucose affinity of two temple-like macrocycles toward octylglucose in chloroform using molecular dynamics (MD) simulations. We then examine their water-soluble versions, solubilized by the addition of large nanocarboxylate groups. According to our findings, we anticipate embedding a stable and precisely designed cavitand along with attractive functional groups enhances the glucose affinity of these dynamic binders. Accomplishment in the implementation of dynamicity to a suitable glucose binder can revolutionize the treatment of diabetes.

Computational Study and Design of Underwater Adhesives Dylan Fortney, Purdue University

Adhesives are ubiquitous materials found in a wide range of applications and thus need to be adaptable to a similarly wide range of surfaces and environments. Current materials that retain adhesive strength underwater are based on the catechol moiety, first identified in marine mussels and other forms of aquatic life. These adhesives are unique in their demonstration of both strong adhesion and bulk cohesion in aquatic environments. While the adhesive strength of these materials is the subject of much experimental work, the mechanism allowing for underwater adhesion is poorly understood. Here, computational study of catechol and chemically similar molecules investigates the molecular-level effects driving adhesion in aqueous environments. Steered Molecular Dynamics (SMD) simulations were performed on candidate molecules to calculate the favorability of each molecule attaching to an alumina surface. The resulting free energy of binding curves showed that catechol-based molecules performed the best, with additional hydroxyl groups yielding additional adhesive benefits. Visual and numeric analysis of these trajectories showed that water binds tightly to the alumina surface, with the strongest adhesive groups binding to this surface-bound water layer, the surface itself, and in some cases both simultaneously. Density Functional Theory (DFT) was used to calculate the oxidation potential of each molecule to compare cohesive strength, which showed that catechol groups had moderate oxidative potential compared to other molecules tested. The results from preliminary molecules were used to inform the design of additional molecules, which were tested on the same metrics. The additional molecules tested reaffirmed the benefit of adding hydroxyl groups, as well as the sensitivity of adhesion to binding atom geometry. Overall these results indicate that underwater adhesion is significantly driven by molecular ability to replace multiple water molecules, with stronger adhesives being able to replace two or more water molecules at the surface or at the surface-bound water layer. This gives a simple and effective design rule for the development of improved underwater adhesives in the future.

Single-Layer Neural Network Model for Platinum Oxide Formation Veronica Freund, University of Notre Dame

Metal oxides have a variety of applications in energy storage and catalysis. Various platinum oxides have been found to exhibit electrical conductance in 1 or 2 dimensions, a property not found in most other oxides. These oxides are synthesized at high temperatures and some of them, such as Pt3O4, are only stable at temperatures around 900K. Because doing experiments at these temperatures is challenging, investigation of the growth and behavior of these phases through molecular dynamics simulations would be a valuable tool in verifying the structural composition and method of synthesis for various oxides. We are using machine learning (ML) to generate a potential energy surface and force field for Platinum and Oxygen which accurately models the formation of Platinum Oxides.We are utilizing the Neuroevolution Potential (NEP) machine-learning framework built for molecular dynamics applications. This framework includes radial and angular descriptors that generate the input layer using the atomic coordinates in each configuration. The training and testing data was generated using Car-Parinello method planewave dft calculations with a non-empirical ultrasoft PBE pseudopotential. The data samples 300 frames each of Pt, PtO, PtO2, PtO3, Pt3O4, two configurations of O2 molecules and two crystallized oxygen unit cells all of which started with crystal structures sourced from Materials Project. Additional frames of adsorption of O2 onto the Pt-111 surface, Oxygen atoms forming O2, and movement of O3 molecules were created manually and added to the dataset. Our current model in the NEP framework maintains stable bulk and surface structures for Platinum as well as providing correct surface energy. Larger heterogeneous simulations using our current model form stable O2 and O3 molecules which then adsorb to a Pt surface and partially embed as individual oxygen atoms into the Pt lattice. Use of this model for simulations of the formation of the various platinum oxides would reduce the computation time compared to ab initio simulation and will advance our understanding of the conductance, formation and stability of Pt3O4.

Evaluating the Predictive Accuracy of Tolerance Factors on Chalcogenide Perovskite Metastability Talia Glinberg, University of Minnesota, Twin Cities

Chalcogenide perovskites are a type of ionic semiconductor with the chemical formula ABX_3, where A and B are cations and X is a chalcogen anion—specifically sulfur (S) in this study. These compounds have potential applications in photovoltaics due to attributes such as tolerance to defects and optical absorption in the visible spectrum. Understanding the stability of these structures is a crucial step to discover new materials in this class. This study evaluates the predictive accuracy of classic and recently introduced tolerance factors in determining the thermodynamic stability of ABS_3 perovskites compared with density functional theory (DFT) calculations. Chalcogenide perovskites are less stable in the perovskite structure than their oxide counterparts, which may be due to their enhanced covalent interactions that are not fully captured in the tolerance factors. To explore this, DFT calculations were used to identify ground-state structures, and crystal orbital Hamilton population analysis was used to investigate the nature of bonding, nonbonding, and antibonding interactions. By quantifying covalency in the context of tolerance factors and stability, this work provides insights into the successes and failures of tolerance factors for chalcogenide perovskites. Understanding these limitations will contribute to more efficient discovery and synthesis of new chalcogenide perovskites.

Machine Learning for Thermodynamic Property Prediction Saurabh K Gupta, University of Wisconsin-Madison

This study explores the application of machine learning techniques to thermodynamic property data, building upon prior work that utilised neural networks for direct property prediction. While previous research has demonstrated the efficacy of machine learning in estimating various thermodynamic properties, this work introduces a novel approach: the development of a machine learning classification model designed to predict thermodynamic data behaviour as a function of temperature. This work uses the NIST JANAF data set which used to predict the thermodynamic properties at different temperatures using constants. By shifting the focus from direct property value prediction to temperature-dependent data classification, we aim to provide a more nuanced understanding of thermodynamic behaviour across varying thermal conditions. This classification-based approach offers potential advantages in identifying critical temperature and predicting phase transitions, contributing to enhanced characterisation and optimisation. The results obtained demonstrate the effectiveness of this classification model, highlighting its potential to complement and expand upon existing machine learning-driven thermodynamic property prediction methodologies.

Identifying metal-organic frameworks for trace benzene capture Alexis Halm-Owoo, Northwestern University

This study examines the characteristics of metal-organic frameworks (MOFs) best suited for benzene capture through high-throughput molecular simulations. Capturing trace amounts of benzene from air with a potential to reuse it later provides an environmentally and economically friendly alternative to discarding this harmful waste. We considered two experimentally synthesized MOFs: TCPP and TABPY as a baseline. These structures exhibit high affinity to benzene at ppm levels (10-1000 ppm). The structure of these MOFs was found to be optimal to adsorb benzene, and thus, we used them as a baseline for the high-throughput computational screening. We considered MOFs from the CoRE MOF database to identify candidate structures for enhanced trace benzene capture potential. We performed prefiltering of frameworks by pore size distribution analysis, and the identified MOFs underwent grand canonical Monte Carlo simulations of adsorption, performed with the RASPA code. Investigating four relevant ppm levels (10-10 000 ppm), we identified a number of MOFs that outperformed those reported in the literature. We found informative correlations between the largest cavity diameter (LCD), pore limiting diameter (PLD), and capture performance. This study will assist in a baseline understanding of benzene adsorption and inform further experiential efforts, providing the groundwork for the byproduct's capture and potential reuse.

Effect of Ion Solvation Strength on the Nanoscopic Structure of Single-Ion Conducting Polymer Blend Electrolytes Aidiel Ikmal Abu Hassan, University of Wisconsin-Madison

The growing demand for advanced battery technology has positioned solid-state batteries as a leading alternative to traditional lithium-ion batteries. Single Ion Conducting Polymer Blend Electrolytes (SIPBEs) have emerged as a promising electrolyte candidate; however, their electrochemical performance has yet to meet established benchmarks. Hence, a comprehensive understanding of the nanoscopic structure of SIPBEs is essential to accurately predict their phase behavior and ion transport mechanisms. In this presentation, I will explore the physical properties of a novel class of SIPBEs, which are generated by blending polyethylene oxide (PEO) with an anion-containing methacrylate polymer, (P(MTFSI-X)). Ion-exchange was conducted on P(MTFSI-X) to investigate the influence of K+, Mg2+, Li+, Ca2+ ions on the nanostructure of the SIPBE systems. Furthermore, the molecular weights of the polymers and the ion concentration were varied to elucidate the effects of ion solvation on the phase behavior of these materials. The miscibility of SIPBEs is characterized via differential scanning calorimetry (DSC), while the impact of ion solvation on nanostructure is assessed using small and wide angle X-ray scattering (SAXS/WAXS). Preliminary results indicate that variations in ion solvation significantly influence both the miscibility (blend Tg) and nanostructure (crystallinity and ion-cluster size) of SIPBEs, yielding valuable insights into the thermodynamics and ion transport mechanisms governing these systems.

Controlling Electrostatics and Solvation to Enhance Conductivity in Structured Electrolytes Logan M. Hennes, University of Notre Dame

Solid-state electrolytes are currently being explored as a safe material capable of addressing consumer energy-storage demands. Solid polymer electrolytes, in particular, offer a high energy density and improved safety when compared to liquid-based electrolytes but tend to have a significantly lower ionic conductivity. We hypothesize that structured ionic liquids can enhance conductivity, and we can explore the role solvent has on the performance of these materials through coarse-grained molecular dynamics simulation. These simulations allow us to investigate the solvent's energetic and entropic effects on ion mobility and characterize the transition between mobility modes using the Van Hove self-correlation function. While we observe similar phase behavior (incorporating solid, smectic, and liquid phases) to that seen in experiments, we also observe significantly more mobility in the cationic species compared to the anionic species before the system reaches an arrest transition. We further show how the general results of our study can guide the exploration of materials and target the design of new solid electrolytes with enhanced kinetics and the ability to transport multivalent ions.

Assessing Semi-Supervised Learning Models for Solid-State Synthesizability Prediction Simon Hjaltason, University of Minnesota

A central challenge of inorganic materials design is predicting whether hypothetical candidate materials are synthesizable. Specifically, can precursor powders possibly react to form a given target crystal structure or will that target never be accessible through a solid-state reaction? Computational researchers have explored semi-supervised learning approaches for this task, such as positive-unlabeled (PU) learning, to address the lack of training data on unsuccessful syntheses. We evaluate the performance of several PU learning models to assess how the data used to train these models influences their ability to predict synthesizability. Furthermore, we probe their ability to capture thermodynamic factors such as phase stability or reaction thermodynamics that are physically relevant to synthesis, given the absence of explicit thermodynamic information included in training. Using 1300 materials, we assess synthesizability predictions based on models leveraging both compositional and structural features. For each material, we compare these predictors against each other, the material's decomposition energy (a measure of its stability), and thermodynamic competition heuristics quantifying the formation of other products in synthesis reactions. By analyzing PU learning models in the context of synthesis-relevant thermodynamics, this study aims to accelerate the development of more reliable synthesizability predictors.

Effect of Protective Mutation on Structure & Dynamics of APOE4: A Molecular Dynamics Simulation Study Newton A. Ihoeghian, University of Kentucky

Apolipoprotein E (APOE) 4 is a well-established genetic risk factor for Alzheimer's Disease (AD). Mutations V236E and R251G reduce AD risk, but their molecular mechanisms remain unclear. This study employs molecular dynamics (MD) simulations to analyze how these mutations alter APOE4 structure and dynamics, particularly in lipidation and oligomerization regions. MD simulations of APOE2, APOE3, APOE4, and the APOE4 variants V236E and R251G were conducted over 1000 ns. Results show that both mutations reduce the flexibility of the overlapping lipidation-oligomerization region, making it comparable to APOE2 and APOE3. Additionally, V236E and R251G decrease the surface area of these regions but through distinct mechanisms. V236E predominantly alters hydrophilic regions, inducing more turns and bends. R251G affects both hydrophilic and hydrophobic areas, increasing random coil formations. These structural changes suggest that the protective effects of V236E and R251G stem from reduced flexibility in key functional domains of APOE4, offering insights into potential AD therapies.

Integrating Protein Language Model and Molecular Dynamics Simulations to Discover Antibiofouling Peptides Ibrahim A. Imam, University of Kentucky

Antibiofouling peptide materials prevent the nonspecific adsorption of proteins on devices, enabling them to perform their designed functions as desired in complex biological environments. Due to their importance, research on antibiofouling peptide materials has been one of the central subjects of interfacial engineering. However, only a few antibiofouling peptide sequences have been developed. This narrow scope of antibiofouling peptide materials limits their capacity to adapt to the broad spectrum of application scenarios. To address this issue, we searched for antibiofouling peptides in the vast sequence pool of the microbiome library using a combination of deep learning-based high-throughput search and molecular dynamics (MD) simulations. A random forest-based model with an ensemble of ten independent classifiers was developed. Each classifier was trained by prompt-tuning the foundational protein language model Evolution Scaling Modeling version 2 (ESM2) on a distinct training data set. We constructed the databases containing the same amount of antibiofouling and biofouling peptide sequences to attenuate the bias of the existing databases. MD simulations were conducted to investigate the interfacial properties of six selected peptide candidates and their interactions with a lysozyme protein. Two known antibiofouling peptides, (glutamic acid (E)-lysine (K))15 and (EK-proline (P))10, and one known fouling peptide, (glycine)30, were used as the reference. The MD simulation results indicate that five of the six peptides present the potential to resist biofouling. Our research implies that deep learning and molecular simulations can be integrated to discover functional peptide materials for interfacial applications.

In silico exploration of metabolite-derived soft materials using a chemical reaction network: what is possible? Shruti Iyer, University of Illinois, Urbana-Champaign

The current materials industry, spanning plastics, fuels, fabrics, and other consumer products relies on chemical building blocks obtained from petroleum feedstocks. The depletion of crude oil reserves and their associated adverse environmental impacts necessitate the exploration of innovative sourcing strategies for functional organic material synthesis. Microbial metabolites derived from biological sources offer promising alternatives for chemical synthesis, but their suitability for soft materials applications remains largely unexplored. We constructed a chemical reaction network integrating databases of common microbial metabolites, E. coli, S. cerevisiae and P. aeruginosa, with the USPTO reaction dataset to examine what is possible in the chemical space of metabolite-derived chemistries of relevance to soft materials. Our analysis revealed that each organism produces a distinct set of unique metabolites with varying structural diversity, with the accessible space saturating rapidly within three synthetic steps from the original microbial metabolites. Moreover, we identified overlaps between the chemical space accessible from metabolite precursors and key petrochemical building blocks, known and proposed synthetically feasible polymer monomers, and the chemical space of common organic electronics and redox active materials. Overall, this work introduces a computational framework for exploring a novel paradigm of soft materials discovery with the potential to accelerate the identification of soft materials relevant to metabolic engineering targets and non-petroleum sourcing pathways for existing soft materials.

Dissecting differences in how chromatin-associated proteins modulate the stability and folding of nucleosome arrays using CG simulations Utkarsh Kapoor, University of Wyoming

The three-dimensional organization of chromatin is shaped by nucleosome interactions and chromatin-associated proteins, yet how different proteins influence chromatin folding and stability remains unclear. Using our high-resolution sequence-specific coarse-grained protein and DNA models in molecular dynamics simulations, we examine how histone H1, heterochromatin protein 1 (HP1α) dimer, and a truncated Polyhomeotic (PHC3) protein affect the stability and folding pathways of tetra- and hexa-nucleosome arrays. These proteins have distinct chromatin-associated functions, but the mechanistic differences in how they modulate nucleosome interactions and chromatin architecture remain poorly understood. Our simulations aim to determine whether these proteins stabilize, disrupt, or reorganize the characteristic α-tetrahedron and β-rhombus conformations observed in chromatin fibers. By comparing their effects on chromatin compaction, flexibility, and structural transitions, we seek to uncover how these proteins differentially regulate chromatin folding.

Mechanism of an Enthalpically-Driven DNA Minor Groove Binding Process from Weighted Ensemble Simulations Nell E. Karpinski, University of Notre Dame

Distamycin is a naturally occurring antibiotic and a DNA minor groove binder. It is also the first minor groove binder discovered to bind in a 2:1 antiparallel motif and is used as a template for designing other minor groove binding ligands. Distamycin binds preferentially to DNA sequences containing adenine (A) and thymine (T) rich tracks, and the binding of distamycin to DNA is enthalpy driven in the 1:1 and 2:1 binding modes. Although distamycin is highly studied, a comprehensive understanding of the binding mechanism of distamycin to DNA has yet to be achieved. To investigate the underlying 1:1 and 2:1 binding mechanisms of distamycin to d(GTATATAC)2, we performed atomistic resolution molecular dynamics simulations applying the weighted ensemble (WE) enhanced sampling method. We obtained an ensemble of trajectories for each binding mode, and we found distamycin binds more concertedly in 2:1 than in 1:1. In contrast, in 1:1, around 45.2% of trajectories exhibit a slow formyl minor groove association once the amidino group has begun insertion. In addition, we observe a dehydration of the minor groove upon 1:1 binding and a minor groove width expansion upon 2:1 binding.

A Robust Force Field for Perfluorooctanoic Acid: Predicting Vapor–Liquid Equilibria
Aastha Kasera, Northwestern University

Per- and polyfluoroalkyl substances (PFAS), known for their thermal stability, durability, and surfactant properties, have seen widespread industrial use over the past few decades. However, the persistence of these “forever chemicals” in water and their alarming health effects have prompted regulatory agencies, such as the U.S. Environmental Protection Agency (EPA), to set maximum contaminant levels as low as parts per trillion. To accurately study PFAS capture at the molecular level, a well-defined force field is required. While existing literature provides some force fields for PFAS molecules, they lack some parameters and are unvalidated against experimental data. In this work, we are developing a robust and reliable force field for one of the most studied classes of PFAS, per- and polyfluoroalkyl acids (PFAAs), starting with perfluorooctanoic acid (PFOA). We have used ab initio calculations to parameterize the torsional potentials and partial charges. To test the force field, we have performed Gibbs ensemble Monte Carlo simulations to calculate the critical parameters, enthalpy of vaporization, boiling point and bulk density and comparing them to experimental values available in literature. We have also performed preliminary simulations using our force field to investigate the adsorption behavior of MOFs for PFAS removal from water. We calculate Henry’s constants of PFOA and water in various experimentally studied MOFs for PFAS capture to evaluate their relative affinities and investigate their potential in removing PFAS from water in dilute conditions.

Data-Driven Design and Screening of Green Solvent Mixtures for Liquid-Phase Chromatographic Separation of Lignin Monomers Changsu Kim, Univ. of Wisconsin-Madison

Lignin serves as a renewable feedstock for aromatic monomer production, offering a sustainable alternative to petroleum-based chemicals in industrial manufacturing. Separation of monomers is a critical hurdle for lignin valorization because lignin depolymerization produces a complex mixture of monomeric products. Centrifugal partition chromatography (CPC) is a promising liquid-phase separation technology that can effectively isolate individual monomers from this crude mixture based on differences in their logP values, which reflect the different tendencies of individual monomers to partition into two immiscible phases formed in a solvent mixture. While halogenated solvents such as dichloromethane have been employed successfully to separate lignin monomers using CPC, these solvents are hazardous due to the high toxicity, motivating the development of green solvent mixtures. A central challenge in designing green solvent mixtures to fully replace halogenated solvents lies in navigating the vast possible solvent design space to identify solvent mixtures that achieve suitable logP values for the target products. In this research, we propose a data-driven approach to optimize solvent selection for lignin monomer separation by CPC by elucidating the design rules of green solvent mixture. A logP value prediction model was developed by using artificial neural networks (ANNs) trained on experimental datasets on aromatic monomer separation with green solvent mixtures. The experimental datasets include five aromatic monomers–pHBA, syrinaldehyde, syringic acid, vanillic acid, and vanillin–paired with eight solvents–heptane, ethylene glycol, ethyl acetate, diphenyl ether, ethanol, dimethyl adipate, methanol, and water. The experimental datasets are represented by the physiochemical properties and Hansen solubility parameter-weighted volume ratio of solvent mixture for monomers and solvent variables, respectively. The approach requires identifying the phase behavior of each potential solvent mixture to screen out miscible solvent systems and estimating the relative volumes of immiscible phases. The reliability of the logP prediction model is then evaluated by K-fold cross-validation as well as leave-N group out cross validation with test datasets. Moreover, the extrapolation capability of the logP prediction was tested on the monomers (e.g., methyl paraben, isoeugenol, ethyl phenol) with a variety of lignin sources (hardwood, softwood, and herbaceous). Our approach can (1) accelerate the experimental discovery of green solvent mixtures via inverse engineering strategies, and (2) promote sustainable lignin valorization by identifying optimal green solvent mixtures for monomer separation.

Aggregation and Cluster Composition in Latex-Pigment Mixtures: A Molecular Simulation Study Ashley Knoerdel, University of Illinois Urbana-Champaign

Colloidal suspensions have many applications, for example paints and coatings. Using molecular dynamics simulations, we aim to provide fundamental molecular-level insight into the formation of composites and aggregates in high-end latex-based coatings. The paint suspension is composed of latex and multilayered pigment particles, as well as dispersants and other additives. This complex mixture complicates the cross- and self-interactions of all components, thus affecting aggregation. We provide insight into the properties of paint coatings by investigating the interactions that affect the aggregation and formation of small clusters in suspension. We vary the amount of latex compared to pigment in the system, the total volume fraction of latex and pigment, and the strength of the cross- and self-interactions. Using simple physical models for effective interactions between particles, we elucidate how the propensity to aggregate and the local latex-pigment environment changes. We also investigate cluster fractal dimension, composition, and kinetics.

Simulating the Flow of Polymer Solutions in Taylor-Couette Geometries
Tzortzis Koulaxizis, University of Illinois Urbana-Champaign

In this study we investigate the behavior of dilute polymer solutions in various geometries. To simulate polymers in good solvent conditions, we utilize molecular dynamics simulations of Kremer-Grest model polymers coupled with Multi-Particle Collision Dynamics (MPCD) to capture hydrodynamic effects. Simulations were conducted primarily in Taylor-Couette channels. We first validate our approach by determining the viscosity of the MPCD fluid and by simulating the flow of the pure Newtonian solvent and comparing our simulations to an analytically predicted flow field. We then characterize the polymer conformations and flow of the non-Newtonian polymer solutions in the same geometry, aiming to identify signatures of turbulence. Our simulations have important implications for understanding processes involving flow through porous media, such as enhanced oil recovery and environmental remediation.

Identifying driving forces of polymorphic bacterial microcompartment assembly through multiscale simulations Emiel Kram, Colorado School of Mines

A key challenge in metabolic engineering is increasing the yield of desired chemicals, which is hindered by the dispersed organization of key enzymes, substrates, and intermediates. Bacterial microcompartments (BMCs) offer a potential solution by encapsulating metabolic processes within a semi-permeable nanoreactor. Similar to viral capsids, BMC shells consist of monomers organized into oligomeric subunits where each subunit is permeable to selective substrates. Engineering the shell morphology and subunit stoichiometry has been shown to alter shell substrate flux and, consequently, the metabolic function of the BMC. However, studies have observed polymorphism in BMC assemblies under fixed conditions, which highlights the uncertainty in how BMC subunit interactions precisely control the shell morphology and stoichiometry. Here, we present two complementary narratives that elucidate BMC assembly mechanisms: subunit-subunit interface binding and collective self-assembly. We focus on three types of BMC monomers from bacteria Haliangium ochraceum: BMC-H (hexamer), BMC-T (trimer), and BMC-H2 (pseudo-hexamer). Structurally, BMC-T and BMC-H2 consist of tandem copies of BMC-H connected by a different peptide linker, respectively. When expressed individually, BMC-H and BMC-H2 assemble into rosette sheets and 25 nm icosahedral shells, respectively. Conversely, BMC-H and BMC-T jointly assemble into larger 38.5 nm icosahedral shells. We present an all-atom molecular dynamics (MD) workflow that employs enhanced sampling and data-driven collective variable discovery to investigate how conformational motions affect the binding pathways and binding free energies between combinations of BMC-H and BMC-T subunits. We also present bottom-up coarse-grained (CG) MD of BMC-H and BMC-H2 to identify molecular factors (i.e., subunit interaction strengths and linker rigidity) that dictate the polymorphic assembly of these monomers, including experimentally observed structures.

Computational Modeling Approaches for Optimizing Mineral Removal from Biomass
Jung Min Lee, University of Wisconsin-Madison

Mineral removal through chemical leaching is a crucial step to improve the efficiency and stability of biomass conversion processes. While dilute acid washing effectively removes both loosely and tightly bound inorganics, its optimization remains challenging due to the complex interactions between mineral species and biomass matrices. To address these challenges, an integrated computational framework that combines geochemical modeling and molecular dynamics (MD) simulations was employed. Specifically, since there has been no prior research on mineral phase diagram modeling and MD modeling for biomass mineral removal, the proposed research will provide a valuable foundation for future work in this area. First, mineral phase diagrams using Geochemist's Workbench (GWB) were constructed to predict solubility limits under various conditions (temperature, pH, acid type), based on tabulated Gibbs free energies of mineral phases. These diagrams help identify favorable thermodynamic windows for mineral dissolution. Second, MD simulations are used to compute molecular-level descriptors including solvation free energy, ion diffusion coefficients, and binding affinities of leaching agents to biomass-associated minerals. These insights help quantify kinetic and thermodynamic barriers to mineral removal, especially for tightly bound or insoluble species like silica. By incorporating MD-derived parameters into geochemical models, we enhance the predictive capabilities of phase diagrams and validate thermodynamic predictions under biomass-relevant conditions. This integration also allows us to distinguish whether mineral removal is limited by intrinsic dissolution kinetics or by transport through the porous biomass matrix. Overall, this framework can be used to develop selective, stepwise pretreatment strategies, such as sequential acid treatments or combined chelating and acidic leaching, that achieve high mineral removal efficiency while minimizing loss of biomass organic matrix. Ultimately, this work is expected to support the design of more efficient and sustainable biomass pretreatment systems through predictive modeling tools that reduce trial-and-error experimentation.

The Effect of Mixed-Mechanism Bond Exchange on Dynamic Network Rearrangement
Min-Hsien Lin, University of Illinois at Urbana-Champaign

Covalent adaptive networks (CAN) are characterized by their thermally responsive topologies and self-healing properties due to the presence of dynamic bonds that serve as crosslinks. CANs can be classified into dissociative or associative networks, depending on how the dynamic bonding mechanism leads to topological rearrangement; dissociative crosslinks break and re-form, and associative crosslinks undergo bond exchange. The latter leads to more robust materials, but the former is easier for reprocessing. Mixed-mechanism networks have the potential to possess both characteristics, in particular, in the situation that dissociated bonds generate free reactive sites that can also participate associative reactions. In this study, we use coarse-grained simulation to understand the relationship between bond energies and binding barriers for mixed associative-dissociative CANs. The presence of free reactive sites governs the bond lifetime of dynamic covalent bonds, indicating that the relaxation dynamics of CANs can be tailored through precise molecular design. By analyzing the diffusion coefficient of free reactive sites, we can gain deeper insight into the relationship between the number of free reactive sites and the facilitation of bond exchange. Furthermore, the mechanical properties of mixed associative-dissociative CANs can be elucidated by examining their stress relaxation behavior, which reveals how the dynamic exchange of bonds contributes to overall material performance. This study aims to provide molecular-level insights into the dynamic bond exchange and cross-link rearrangement by examining the bond lifetime and the dynamics of free reactive sites, enabling the rational design of CANs with tunable properties for future applications.

Stepwise Chemical Discovery for Stable Organic Radicals Yun-Ke Liou, Purdue University

Stable organic radicals represent a novel class of organic materials characterized by the presence of an unpaired electron, which plays a crucial role in energy storage and conversion applications. Specifically, the reduction-oxidation activity of stable organic radicals enables energy storage in organic batteries, while the accessibility of the doublet state facilitates photovoltaic energy conversion. Despite their broad applicability, the knowledge of stable organic radicals remains limited to a small number of known species, as most radicals only transiently exist for the high reactivity. In this study, we aim to devise and implement a Genetic Algorithm for optimizing molecular structures to discover new stable organic radicals.

The Genetic Algorithm initially samples new radicals on molecular graphs. The sampling process employs mutation to modify the atomic types and connectivity or the crossover operator to recombine molecular fragments by functional group exchange. Subsequently, a fitness evaluation is performed using quantum chemical calculations to assess the thermodynamic and kinetic stability of the newly generated radicals. In each generation, only the top-scored candidates are selected, and the next population is derived from these elite molecules. The iterative optimization process continues until a set of best radical scorers is identified.

Preliminary results indicate that the Genetic Algorithm not only successfully navigates between various known radical classes but also converges toward an increasingly refined search space. Moreover, the evolution strategies of transient radicals show the tendency to develop five- and six-member ring structures along with steric protection to ensure stability. These findings establish a proof-of-concept for the application of Genetic Algorithms in the discovery of stable organic radicals, demonstrating the potential for automated radical design.

Unexpected Chemi-/Physisorption of CO2 on Zirconium Metal-Organic Frameworks through Halide-Functionalization and its Impact on Carbon Capture Jiayang Liu, Northwestern University

In recent decades, the widespread release of CO2 into the atmosphere has gained significant attention due to its impact on the climate, ocean acidification, etc. In light of this, carbon capture and storage (CCS) has emerged as a tool to tackle the CO2 emissions from electricity production and industrial manufacturing. Metal-organic frameworks (MOFs), a type of crystalline structures featuring tunable nanopores are a promising class of adsorbents for carbon capture.

Zirconium-based MOFs are known for their excellent hydrothermal stability and highly tunable node surfaces. Previous studies have shown that the Zr-MOF NU-1000 is a robust platform for node functionalization through solvent-assisted ligand incorporation (SALI) and other post-synthesis treatments. In this study, we explored three forms of Zr-MOFs, formate-capping, aqua/hydroxyl ligand-paring, and charge-compensating halides. We unexpectedly found a competition between CO2 chemisorption and physisorption with the zirconium nodes and explained the observation with DFT calculations. We explored the impact of different node functionalization on carbon capture using grand canonical Monte Carlo (GCMC) simulations and investigated how water molecules interact and cause hysteresis inside the pores using transition-matrix Monte Carlo (TMMC) simulations considering the wet flue gas conditions. The use of these simulation tools enables us to gain a deeper and comprehensive insight into Zr-MOFs and design rules for new materials for optimal carbon capture.

Material Property Changes Influence Cancer Progression Mechanisms Hailey Lynch, University of Notre Dame

Underlying mechanics such as increased stiffness and degradation of the extracellular matrix (ECM) influence the remodeling processes that promotes cancer progression. Since the ECM is tumor-specific, understanding the contribution of material properties such as viscoelasticity towards changes in the tumor microenvironment is urgently needed. Here we propose to incorporate viscoelasticity (i.e, naturally occurring property of biological tissues) in a tumor model to describe the impact of material property changes during cancer progression. We look to understand the viscoelastic influence as it relates to modeling systems comprised of soft matter such as cancer within the brain.

Computational Exploration of Degradation Pathways of PBX Polymer Binders Andrew Marquardt, Notre Dame

The hydrolytic degradation of Estane, a poly(urethane ester), has been studied extensively to determine dominant degradation reactions and accurate kinetic models at a variety of temperatures, humidities, and pH. These experiments have provided extensive data for the creation of accurate models, but often stretch over multiple decades due to the high stability of the material in mild conditions. By utilizing Yet Another Reaction Program (YARP), a computational reaction enumeration and transition state search algorithm, high-throughput computing was leveraged to study this degradation behavior in a fraction of the experimental time. All experimentally relevant degradation reaction pathways were identified, enabling qualitatively accurate determination of relative reaction rates on the order of months. This study demonstrates the potential of YARP to aid in materials analysis by significantly decreasing the time required to identify relevant reactions of interest in commonly-encountered environments.

Evaluating strategies for enhancing efficiency of machine-learned interatomic models for condensed phase reacting systems Emeline Martin, University of Michigan

Machine-learned interatomic models (ML-IAM) have gained significant interest as a means of achieving “quantum accurate” atomistic simulations. However, in systems with strong dispersion interactions, these models are costly due to the need to describe both short- and long-range (e.g., bonded and non-bonded) interactions. In this work, we show that ML-IAM expense can be significantly reduced without compromising on accuracy by training models to only the short-ranged portion of the interaction range and including an empirical dispersion correction. We demonstrate that using this approach, we can generate efficient models using the Chebyshev Interaction Model for Efficient Simulation (ChIMES) to model nitrogen under extreme-temperature and high-pressure conditions that are as accurate as those generated through the more expensive standard fitting scheme.

ChIMES Machine Learning Interatomic Potential for Water under Extreme Conditions Using a Hierarchical Transfer Learning Approach Poornima Moremada, University of Michigan

Water under extreme thermodynamic conditions exhibits complex phase behavior, particularly in the superionic regime relevant to the interiors of planets like Uranus and Neptune. In these environments, water can form exotic phases characterized by high hydrogen diffusivity within a crystalline oxygen lattice, occurring at pressures above 400 GPa and temperatures around 5000 K. Despite the importance of these phases, many aspects of the phase diagram and thermophysical properties of superionic water remain uncertain.

Interatomic potentials (IAPs) provide a computationally efficient pathway to explore these regimes.

However, developing machine-learning-based IAPs (ML-IAPs) for highly dense reactive systems, such as water under extreme conditions, remains a complex and time-intensive task. To address this, the present study explores a hierarchical transfer learning approach within the ChIMES machine-learned interaction potential framework for modeling water under extreme conditions. This approach leverages parameters optimized for pure hydrogen and oxygen to improve both accuracy and consistency in the combined H/O model.

Model development is further streamlined by the ChIMES Active Learning Driver (ALDriver), which systematically identifies and corrects high-error regions in the training dataset. Moreover, it lays the groundwork for extending the model to systems composed of the same elemental subsets such as pure O2 or H2 offering critical insights into the broader applicability of the hierarchical transfer learning strategy.

Detection of Relaxation Events in Supercooled Liquids using Topological Data Analysis

Angan Mukherjee, University of Wisconsin-Madison

Topological data analysis (TDA) is a powerful tool for extracting information from complex datasets. In recent years, TDA has found remarkable success in diverse applications, spanning neuroscience, materials science, and network analysis. In this work, we show that TDA is a robust, scalable, and interpretable method for detecting relaxation events in supercooled liquids. We also show that TDA provides understanding of the complex spatio-temporal heterogeneous dynamics (i.e., across time and across spatial locations of the process). The focus on connectivity is a key defining aspect of TDA over other conventional methods used for event detection such as principal component analysis, convolutional neural networks, autoencoders, support vector machines, and Fisher discriminant analysis. TDA also offers robustness, as topological descriptors remain invariant under certain types of perturbations such as scaling, rotation, and random noise. Moreover, TDA computations are significantly more scalable than other approaches such as convolutional neural networks.

We use electron correlation microscopy (ECM) to generate experimental data by probing supercooled liquid dynamics beyond ensemble-averaged measurements. ECM enables the study of individual mobility events via two-time correlation function (TTCF), thus revealing their distinct behaviors and characteristics. We explore different representations of the TTCF data obtained from ECM experiments as images and manifolds. We then use basic topological descriptors to identify 'topological signatures' that point towards the types, durations, and frequencies of occurrence of relaxation events in supercooled liquids. Moreover, we show how a combination of TDA and clustering approaches identify a low-dimensional latent space of the process that helps visualize the onset and dynamics of diverse event types.

Expanding Cluster, Enhancing Adsorption: Investigating the Role of Electrostatic Configurations on Water Vapor Adsorption in Idealized Nanoporous Materials

Krishnendu Mukherjee, University of Notre Dame

Understanding and tuning water vapor adsorption at nanoscale can inform technologies such as atmospheric water harvesting, dehumidification, water-energy nexus design, etc. Porous materials have shown great promise as water adsorbents with studies revealing how different adsorbent properties such as functional groups, pore size, surface charge, etc. can influence adsorption. However, recently it has been shown that patterning or configuration of interacting sites are equally important in water dynamics (diffusion) and water-protein interactions. Present research work engages with this question: can electrostatic configuration influence water vapor adsorption? In this work, continuous fractional component grand-canonical Monte Carlo (CFC-GCMC) is applied to perform water adsorption simulations in idealized cylindrical nanopores for five different charge configurations with varying pore size (1, 1.1 and 1.2 nm) and charge magnitude ($+/-$ 0.39-1.17). The alternating along (AA) configuration (positive charges in the inner ring and negative in the outer ring while alternating in z-direction) demonstrates higher water uptake at saturation and water adsorption starts at a much lower pressure than other configurations. Analysis of water clustering pattern in AA reveals radial as well axial expansion of water clusters which facilitates accommodation of extra water molecules. Increasing charge magnitude shifts the type-V isotherm inflexion point leftwards along the pressure axis, thereby increasing the hydrophilic nature of the AA configuration. Probing different energetic interactions and electrostatic potentials of the configurations suggest unique relaxation of the water clusters in the AA patterned cylinders. Investigating the effect of charge magnitude and pore size provides more evidence to their hydrophilic nature. Finally, analyzing the hydrogen bonding and adsorbed phase characteristic at saturation hints at strong ordering induced by the pore confinements and the electrostatic configurations compared to bulk liquid water. The simulations show that tailored charge arrangements can enhance adsorption by facilitating uptake at lower pressure as well as achieve higher water capacity at saturation.

Understanding the mechanism of action of human growth hormone antagonist using molecular simulations Hemant Nagar, Ohio University

Human growth hormone (hGH) is a peptide hormone composed of 191 amino acids secreted in the pituitary gland. Interaction between growth hormone and its receptor (GHR) plays a pivotal role in various physiological processes, including growth, metabolism, immune function, and cell regeneration in humans. Abnormal secretion levels of hGH can lead to conditions, such as acromegaly, characterized by excessive hormone levels. Dr. Kopchick's lab developed GHR antagonist, which blocks the normal action of the hormone by making a point substitution of Glycine 120 to Lysine on the native protein. This GHR antagonist is commercially marketed as Somavert drug by Pfizer. We are interested in studying the binding mechanism of growth hormone antagonist to receptor in comparison to the native one. For this, we have employed the Umbrella Sampling technique. Our simulations revealed that interactions between antagonist with receptor is different from the native one. Additionally, we have conducted the Alanine scanning mutagenesis on native growth hormone to identify the sites that can be substituted with other amino acids to make the more potent antagonist.

Effects of cardiolipin and branched-tail lipids on properties of model chlamydial membranes Nikhil Nambiar, University of Tennessee,, Knoxville

The bacterium Chlamydia trachomatis divides via a polarized budding process. This is in contrast with most other bacteria, which divide via binary fission. Cardiolipin synthase, which catalyzes the production of the four-tailed lipid cardiolipin, was observed to be enriched at the budding site. The enrichment of cardiolipin at the budding site is believed to be a key feature in facilitating cell division in chlamydia, but it is unclear how it modulates properties of the membrane. Moreover, lipidomic analysis has shown that the most abundant lipid tails in chlamydial membranes are iso- or anteiso-methyl-branched saturated tails. However, the effect of tail branching on bacterial membranes has not been studied extensively. In this work, we use all-atom molecular dynamics simulations to investigate the effects of cardiolipin and lipid tail branching on the properties of model chlamydial membranes. Our results demonstrate that the addition of branched-chain lipids introduces disorder in the membrane, inducing a monotonous decrease in bending rigidity. This is accompanied by a decrease in membrane thickness and increase in area per lipid, suggesting a transition from gel phase to liquid phase. The addition of cardiolipin was observed to increase bending rigidity of membranes with branched-tails, while mildly decreasing the bending rigidity in membranes with straight tails. This suggests that cardiolipin might be recruited at the budding site to induce curvature rather than reduce bending rigidity. These findings highlight the importance of incorporating both tail branching and cardiolipin distribution when developing models of chlamydial membranes.

Brownian Bridges for contained random walks
Vivek Narsimhan George Curtis Doraiswami Ramkrishna, Purdue University

We demonstrate an efficient method to investigate rare events in stochastic processes. Specifically, we examine rare event trajectories which lie at the tail end of the first passage time distribution, whose survival time is much greater than the mean escape time within a specified domain. We do this by generating contained trajectories, which are continuous random walks that only stay within a specified region of phase space for at least a set period of time T. These trajectories are efficiently generated using a Brownian Bridge, which is constructed from the solution Backward Fokker-Planck (BFP) equation. Using linear operator techniques, we show that the BFP operator can be placed into self-adjoint form and in the asymptotic limit, T much greater than 1, the set of contained paths is equivalent to the trajectory ensemble of paths on a modified potential energy landscape which depends solely on the dominant eigenfunction of the BFP operator. We demonstrate this idea in several examples, including the Graetz problem, where we examine a particle diffusing in tube flow and show an exponential increase in simulation efficiency in comparison to brute force sampling.

Boosting Hybrid 2D Perovskite Stability Through Computational Screening of Ligand Chemistries Zhichen Nian, Purdue University

2D hybrid perovskite materials are attractive from the perspective of providing a much larger design space of organic ligand chemistries in comparison with bulk 3D materials. Likewise, many recent reports have highlighted how tuning the ligand chemistry can impact the electronic properties and stability profiles of the resulting 2D materials. In this talk, we'll describe how we have implemented a high-throughput molecular simulation framework to screen prospective ligand chemistries for synthesizability and stabilization of the perovskite lattice. ML models have been also incorporated to accelerate the prediction. Using this framework, we have been able to characterize thousands of perovskite materials and establish some novel design rules for ligand chemistries. Several novel aspects of the methodology will also be highlighted, including extending our screening approach to elucidate differences in design rules with transitioning from 2D to Quasi-2D perovskite.

Modification of Machine Learned Interatomic Potential Design Architecture to Increase Simulation Efficiency Awwal Oladipupo, University of Michigan

In recent decades, atomic-resolution simulation for materials modeling has become integral for tackling challenges such as climate change and power inefficiencies by reducing experimental trial-and-error. Recently, researchers have turned to machine-learned interatomic potentials (ML-IAPs) to accelerate these endeavors, since they can serve as an efficient proxy for quantum-based methods capable of material simulations at orders of magnitude greater spatiotemporal scales.

Nevertheless, ML-IAPs face limitations, e.g., struggling to accurately capture long-range interactions and exhibiting a greater computational expense relative to classic force fields, making the exascale simulation needed for describing many complex phenomena largely out of reach. In this study, we developed a multilayered ML-IAP to meet these challenges. This strategy drives down simulation costs by up to 93% compared to standard approaches, enabling quantum accurate simulations on experimentally relevant scales, toward insights that advance our understanding of materials and chemical sciences.

Context-Dependent Hydrophobic Interactions of α-Peptides ByungUk Park, University of Wisconsin-Madison

Hydrophobic interactions are water-mediated attractions between nonpolar molecules or surfaces. These interactions provide the driving force for many self-assembly and molecular recognition processes, such as receptor–ligand binding, protein folding, and the formation of lipid assemblies (e.g., vesicles). Nonpolar surfaces in biological systems are not exposed in isolation but are typically flanked by a diverse range of uncharged polar and/or ionic groups. While nonpolar surfaces are the major entities that mediate hydrophobic interactions, recent experimental studies using atomic force microscope (AFM) measurements suggest that the hydrophobic interactions of α-peptides vary depending on the flanking ionic group identity. Seeking to understand how hydrophobic interactions of α-peptides vary depending on sequence features and chemical context, we modeled α-peptides that share identical amino-acid sequences except their charged residues (lysine or arginine) and can fold into globally amphiphilic helices. We performed all-atomistic molecular dynamics simulations, steered molecular dynamics, replica exchange, umbrella sampling, and metadynamics to characterize mechanistic and energetic differences in the interactions between these peptides and a uniformly nonpolar surface. This work reveals that changing the flanking ionic group identity can significantly change the hydrophobic interaction patterns and such differences are attributed to the sequence-encoded secondary structure of the peptides in aqueous conditions. Analysis of local water structure adjacent to nonpolar domains of the α-peptides shows that propagation of perturbations to solvent structure is marginally different depending on the ionic group identity. Overall, our results highlight the complexity of the noncovalent networks that govern intermolecular associations and point out the inability of context-independent measures (e.g., hydropathy scales) to completely quantify hydrophobicity patterns on a protein surface.

Modeling Side-Chain and Salt Effects on Carrier Mobility in Conjugated Polyelectrolytes Huihang Qiu, University of Illinois Urbana Champaign

Conjugated polyelectrolytes (CPEs) exhibit dual ionic and electronic conductivity, making them promising candidates for optoelectronic, biosensing, and energy-harvesting applications. However, the structure-property relationship in CPEs remains underexplored due to the complex interplay of factors such as side-chain chemistry and salt concentration. This study employs a quantum mechanically informed coarse-grained model, coupled with semiclassical rate theory, to investigate how these factors influence morphology, reorganization energy, and electronic coupling, ultimately impacting carrier mobility. The results emphasize the critical role of torsional energetics in modulating electronic transport in conjugated materials.

A Reactive Monte Carlo-Molecular Dynamics Method for Molecularly Doped Semiconductors Vishnu Raghuraman, University of Illinois Urbana-Champaign

In this work, we develop and implement an atomistic Reactive Monte Carlo-Molecular Dynamics method in order to study doping in organic semiconductors. This method can be integrated with straightforward existing atomistic force-fields and DFT calculations of neutral and doped states, and can explicitly introduce polaronic contributions as well as partial charge transfer. We apply this method to P3HT doped with F4TCNQ, both in the condensed phase and in solvent. We also demonstrate the effect of dopant aggregation on the doping efficiency. This method has been implemented as a fix in LAMMPS and is made publicly available.

Comparison of Hydration Free Energies of Linear Alkanes (C1-C20) and Surfactants in Different Water Models Yalda Ramezani, Ohio University

We have compared hydration free energies of alkanes ranging from methane to eicosane (C20) in different water models (SPC/E, TIP4P2005, OPC, OPC3). We find that hydration free energies estimated using the 4-site water models are closer to the experimental values as compared to those obtained from 3-site water models. We use free energy perturbation methodology in molecular simulations to calculate the hydration free energy. We find that shifting potential functions by the value of the function at the spherical cut-off results in systematic errors in the hydration free energies. We also calculate hydration free energy of cationic and charge-neutral surfactants with different polar head groups. We report that ationic surfactants have a much higher affinity to get solvated in water as compared to charge-neural surfactants. These results reveal the contributions of the polar head and the alkyl tail on the overall hydration free energy, and thus are useful for designing surfactants with the desired aqueous solubility needed for various applications.

Prediction of Second-Order Nonlinear Optical Properties in Metal-Organic Frameworks with Miller Scaling Wilson Raney, University of Notre Dame

In recent years, metal-organic frameworks (MOFs) have been identified as a candidate class of materials for nonlinear optics applications. MOFs are crystalline hybrid materials composed of metal nodes and organic linkers. The design space of MOFs is vast due to the sheer number of node-linker combinations, space groups, and configurations possible. Calculating the second-order nonlinearity of these materials through ab initio methods is computationally expensive and time-consuming. To efficiently and accurately discover new materials suitable for quantum optics applications, new predictive models and methods are needed. One such method, Miller's Rule, is an empirical relationship first proposed in the 1960s that identified a certain ratio between the first- and second-order nonlinear coefficients to be nearly constant. In this work, we assess the suitability of Miller's Rule to predict second-order nonlinearities of nonlinear MOFs. We demonstrate the first known instance of Miller's Rule being applied to a MOF system and explore applying the Rule to anisotropic crystalline systems. These efforts will help to accelerate the progress of computational materials discovery of new MOFs for quantum optics applications.

Guidelines for Open-Source Sigma Profile Generation to Enhance ML Predictions of Thermophysical Properties Fathya Salih, University of Notre Dame

The combination of machine learning (ML) models with chemistry-related tasks requires the description of molecular structures in a machine-readable way. The nature of these so-called molecular descriptors has a direct and major impact on the performance of ML models and remains an open problem in the field. Structural descriptors like SMILES strings or molecular graphs lack size-independence and can be memory intensive. Machine-learned descriptors can be of low dimensionality and constant size but lack physical significance and human interpretability. Sigma profiles (SPs), which are unnormalized histograms of the surface charge distributions of solvated molecules, combine physical significance with low dimensionality and size-independence, making them a suitable candidate for a universal molecular descriptor. However, their widespread adoption in ML applications requires open access to SP generation, which is currently not available.

This work establishes guidelines for generating SPs that enhance ML performance in thermophysical property prediction. Key factors analysed include the effects of the level of theory, COSMO model, SP smoothing, segment size, and conformer selection on the efficacy of SPs when used as inputs to Gaussian Process (GP) models. These insights provide practical recommendations for improving the reliability and predictive power of SP-based ML models.

Phase Behavior and Ion Transport in Lithium-Based Ionic Liquid Crystals
Marvin Diaz Segura, University of Notre Dame

Lithium-based ionic liquid crystals (ILCs) offer a structured approach to electrolyte design for next-generation batteries. Using classical molecular dynamics simulations, we investigate the phase behavior and ion transport properties of Li+C18TFSI- from 300–600 K. Phase transitions are characterized through orientational and translational order parameters and compared to experimental data. We also examine lithium ion conductivity and the effects of electrostatic charge scaling. Our results reveal how mesoscopic ordering impacts ion mobility, providing insights for developing efficient, single-ion conducting materials.

A Statistical Thermodynamic Formulation for Arriving at the Schrödinger Equation: From Classical Diffusion to Quantum Dynamics Yashdi Saif Autul and Subhangshu Sen, Rensselaer Polytechnic Institute

This work presents a first-principles derivation of the time-independent Schrödinger equation from statistical thermodynamics, bridging the gap between irreversible diffusion and the reversible quantum dynamics of an isolated system. Starting from Fick's laws of classical diffusion, we introduce a complex diffusion coefficient, Dq=i$\hbar$/2m, to transform real-exponential decay into sinusoidal, coherent wavefunctions characteristic of isolated quantum systems. This leads to the time-independent Schrödinger equation for a free particle, ensuring dimensional consistency and unitary evolution.

To justify this transition, we analyze entropy dynamics—showing that, unlike classical diffusion which leads to entropy growth, the quantum probability current, being imaginary and phase-driven, preserves entropy over time. We further derive the Schrödinger equation by minimizing a quantum variant of the Helmholtz Free Energy functional using variational principles under normalization constraints - revealing that the quantum behavior emerges naturally from equilibrium statistical mechanics.

Our formulation is validated against Feynman's Path Integral approach via Wick Rotation and the quantum analog of the statistical partition function — thereby establishing formal equivalence between the free-energy-based action and the path integral representation. We extend this thermodynamic framework to relativistic cases, retrieving the Klein-Gordon and maintaining structural similarity to the Dirac equations under similar principles. Conservation laws derived from Noether's theorem also confirm the physical consistency of our model.

This thermodynamic unification offers a novel theoretical lens to interpret quantum mechanics as an entropy-preserving, equilibrium phenomenon - with predictive implications for quantum coherence, reversibility and the structure of quantum statistical ensembles.

Learning Renormalization Group Flows for Lattices Jay Shen, University of Chicago

Real space renormalization is a powerful and theoretically fascinating, albeit difficult technique for investigating scale and phase behavior in physical systems. For even the simplest problems, formulating the so-called renormalization group (RG) flow involves incredibly tedious, intuition-dependent work that can drag on for years. However, once accurately described, RG flows have a number of uses, from describing phase behaviors to speeding up simulations. Accordingly, any information at all about their properties is highly valued and sought after. In this work, we review and assess a novel approach to real space renormalization initially proposed by Hou et al. [1]. The so-called Machine Learning Renormalization Group (MLRG) algorithm automatically determines approximate RG flows of translationally-invariant Ising models, given only the symmetry description of the lattice. It has the potential to effectively characterize a wide range of interesting systems, and also demonstrates an elegant synthesis of both new and old machine learning techniques with statistical physics. Here, we will first give some background for real space renormalization and the Ising model. Then, we will describe the MLRG algorithm and demonstrate its use. Finally, we will discuss the algorithmic design space, propose modifications for improvement, and explore applications to other lattice geometries.

Argon Nucleation in Molten Lithium Chloride Cole Strickling, University of Notre Dame

In this study, we explore the nucleation behavior of argon in molten lithium chloride through advanced simulation techniques. Utilizing the Rigid Ion Model (RIM), which is parameterized from detailed quantum simulations, we employ LAMMPS to simulate the dynamic behavior of argon atoms within the molten salt. This approach allows for the precise calculation of the potential of mean force, providing deeper insights into the likelihood of homogeneous nucleation of argon. Data collection involves rigorous umbrella sampling, subsequently analyzed using the Weighted Histogram Analysis Method to correct for inherent simulation biases. Collaborative efforts with Oak Ridge National Laboratory help validate the RIM's accuracy against ab initio molecular dynamics and a Machine-Learned Force Field. Our findings aim to significantly enhance the understanding of noble gas nucleation processes in molten salts, focusing on the trends and mechanisms of bubble formation.

EPISOL: a fast implicit solvent solver for chemical and biological systems based on 3DRISM theory. Peter Swanson, University of Wisconsin-Madison

Three-dimensional reference Interaction Site Model (3DRISM) calculations are a method for determining solvent density, distribution, and various thermodynamic properties including solvation-free energy. In contrast to extracting these properties from an explicit-solvent simulation which may take hours or days to perform, with 3DRISM, this time can be cut down to a single calculation spanning seconds to minutes. Herein we introduce our 3DRISM software, EPISOL. Compared to existing software, EPISOL shows increased performance, memory usage, and convergence rate alongside an easy-to-use GUI. Our software also includes our recent advances in integral-solvation theory, including hydrophobicity-induced density, and ion-dipole corrections. We provide example calculations spanning biological and material systems containing hundreds of thousands of atoms and compare our results to existing databases.

Simulating Curved Lipid Membranes Using Anchored Frozen Patches James Tallman, University of Illinois Urbana Champaign

Many interesting lipid bilayer phenomena are linked to membrane curvature. Lipid bilayers often form high-curvature configurations due to self-assembly conditions or certain biological processes. However, particle-based simulations of lipid membranes are predominantly of flat lipid membranes because planar membranes are easily connected over periodic boundary conditions. To simulate a curved lipid membrane, one can model an entire vesicle, a cylinder, or a bicelle (a disk-like bilayer aggregate). Alternatively, artificial methods to control curvature are also available, such as applying virtual walls of beads, buckling the membrane, radial harmonic potentials, or "taping up the edges". These existing methods have limitations due to the method by which curvature is imposed. In this work, we propose an alternative method of introducing arbitrary curvature by anchoring a curved lipid membrane with "frozen" equilibrated membrane patches. The method presented here is compatible with all particle-based lipid models and easily extended to many geometries. As an example, we simulate curved membranes with DPPC, DOPC, DLPC and DOPE lipids as parameterized by the Martini3 coarse-grained model.This method introduces limited finite-size artifacts, prevents lipid flip-flop at membrane edges, and allows fluctuations of the free membrane center. We provide verification of the method on flat membranes and discussion on extracting shape and per-leaflet quantities (thickness, order parameter, stress profile) from curved membranes. Curvature produces asymmetric changes in lipid leaflet properties.Then, we explore the coupled effect of curvature and membrane asymmetry in both number and lipid type. Treating the frozen patches as rigid bodies, we show the ability to relax asymmetric membranes to their spontaneous curvature.With imposed curvatures substantially different from the spontaneous curvature of the leaflet, we report the resulting unique morphologies (inducing gel phase, faceting) and behaviors (thickness dependent on adjacent leaflet type) that are accessible with this method.

Dependence of the polymer adsorption transition on chain stiffness and surface interaction range: A partition-function-zero analysis Mark P. Taylor, Hiram College

The reversible adsorption of a polymer chain to an attractive surface is an important problem in materials science and biophysics. The location of this transition (T_c) is sensitive to both polymer flexibility (l_p) and the range of the attractive surface potential (λ) and, for long chains, simple scaling arguments predict T_c l_{pa} λ^b with different power law exponents for different ranges of l_p and λ. Verification of these scaling laws for semi-flexible polymers via computer simulation is challenging due to the long chain lengths required to reach the asymptotic scaling regime. Here we propose a finite-size-scaling method using partition function zeros to obtain adsorption transition temperatures in the long-chain limit from simulations of chains of modest length. By combining the real and imaginary parts of the leading partition function zeros it is possible to eliminate the size/flexibility dependent scaling function that describes the approach, with increasing chain length, of these leading zeros to the critical point in the complex inverse-temperature plane. Our model polymer is a flexible tangent-hard-sphere chain (sphere diameter σ) with a local bond angle restriction that sets a persistence length l_p. The chain is end-tethered to a flat surface that has a square-well attractive potential of range $\lambda\sigma$. We use a Wang-Landau simulation algorithm to obtain the density of states for chains up to length N = 1024 with $1 \leq l_{p/\sigma} \leq 13,000$ and $0.1 \leq \lambda \leq 10$. We distinguish three distinct scaling regimes over this wide parameter space: (i) worm-like chain behavior for $l_{p/\sigma} > max(10, 10\lambda)$, (ii) expanded coil behavior for $\lambda > 1$ with $l_{p/\sigma} < 10\lambda$, and (iii) a single bead interaction region for $\lambda < 1$ with $l_{p/\sigma} < 10$, and we find scaling laws consistent with simple scaling expectations for each of these regions.

RNA Hairpin Folding with Unbiased Weighted Ensemble Sampling Isabel Thompson, University of Notre Dame

Ribonucleic acid (RNA) is a multifaceted molecule essential to cellular life, orchestrating a wide array of biological processes. This versatility stems from RNA's ability to adopt complex 3D structures, assembled from secondary elements like hairpin loops. All atom molecular dynamics (MD) with explicit solvent generates detailed trajectories and dynamic information, however, the de novo simulation of RNA hairpin folding remains a challenge. To overcome technical challenges in the simulation of tetraloop folding due to rough energy landscapes and rare but fast transition events, we apply the weighted ensemble (WE) enhanced sampling method. WE has the potential to capture folding events across rugged landscapes and provide atomistic detail without artificial bias, making it a promising strategy for understanding the biophysical mechanisms of hairpin loop formation at reduced computational cost.

Phosphate Aggregation in Aqueous Solution: Comparison of Non-Polarizable and Polarizable Force Fields Noah Vasconez, University of Notre Dame

We investigated the aggregation of H2PO4- , via hydrogen bonding, in SPC/E water with a full charge, scaled charge, and polarizable AMOEBA force field at variable concentrations. The full charge model yields similar amounts of aggregation to AMOEBA while the scaled charge model shows much lower amounts of aggregation. However, the hydrogen bonded water network in the scaled charge model shows similar behavior to the AMOEBA model. These findings demonstrate that a uniform charge scaling approach to account for molecular polarizability can do well to account for overestimation of ion pairing, but care should be taken when studying systems with significant anion-anion interactions.

Nested Sampling: Advantages and Challenges Ray Yang, Washington University in St. Louis

The nested sampling algorithm has recently shown promise in modeling the phase diagrams of adsorbates on solid surfaces, as a function of temperature and coverage, by directly and efficiently calculating their classical partition functions. Relying only on a minimal set of parameters, nested sampling offers autonomous exploration of phase space without prior knowledge of its stable phases. In this talk, I will compare the performance of nested sampling against established standard approaches—e.g., Monte Carlo sampling and the Wand-Landau algorithm—for determining phase transitions of systems with varying spatial extent and resolution, including continuous Lennard-Jones clusters and solid surfaces, as well as discretized lattice systems. Overall, nested sampling provides the best combination of accuracy, efficiency, and ease of use for small systems (i.e., tens of particles) with continuous particle positions but struggles with lattice systems that have degenerate ground state configurations. I will show how different algorithms can be used in conjunction to achieve more efficient sampling. Finally, I will showcase FreeBird.jl, an extensible toolbox for modeling phase equilibria of atomistic and lattice systems with traditional and modern sampling methods, written in the modern programming language Julia.

Harnessing Molecular Simulation and Modified DLVO Theory for Colloidal Gels to Enhance Battery Electrolytes Caleb Youngwerth, University of Wisconsin-Madison

Despite being contained in nearly every device we use today, current battery design have serious flammability and stability concerns unresolved by commercial electrolyte designs. To address these issues, this study proposes using a colloidal gel within an ionic liquid (IL) as a promising next-generation electrolyte. However, the behavior of these colloidal particles within an ionic solution is still not completely understood. In order to better investigate this behavior, we propose using an improved Derjaguin, Landau, Verwey, and Overbeek (DLVO) theory to allow for massive simulations predicting the aggregation qualities of these gels and topological phase shifts. From there, by using Topological Data Analysis (TDA) and Principal Component Analysis (PCA), we can better quantify these structures to pinpoint these areas of transition. Using these same tools, we also aim to confirm that the modified theory based on recent research findings better describes the characteristics of the colloidal systems.

Predictive Modeling for Gas Adsorption in Metal-Organic Frameworks for Xe/Kr Separation Xiaoyi Zhang, Northwestern University

Xenon has many specialized uses, yet it is extremely rare on Earth, with an atmospheric abundance of only 0.086 ppm by volume. The current production method involves separating it from byproducts of the cryogenic distillation of nitrogen and oxygen from air. This byproduct stream typically contains about 80% krypton (Kr) and 20% xenon (Xe), and further separation requires an additional cryogenic separation, which is costly in terms of both capital and energy. Developing a separation method under mild conditions would facilitate Xe production in a more environmentally friendly way.

A promising class of materials for this application are metal-organic frameworks (MOFs). Previous research has demonstrated the potential of MOFs in gas separation, and many experimental and computational screenings have been conducted on MOF-based gas separation. One challenge in screening MOF structures lies in the extensive simulations required to identify the most selective materials. To address this issue, we are developing machine learning (ML) models as surrogate models. As features in the ML models, we adapted "energy grids," i.e., the potential energy that a probe molecule feels with the MOF framework at grid points throughout the unit cell. We trained and evaluated our model on more than 15000 structures and adsorption data predicted by grand canonical Monte Carlo (GCMC) simulations. Using energy grid features, we employed a Convolutional Neural Network to predict Xe and Kr loadings at six different pressures. Our results indicate that the model can predict Xe and Kr adsorption with high R-squared values compared to the GCMC results across different pressures using a single model. Through the exploration of energy grids for gas separation at various pressures, our research provides a potential pathway for faster screening of MOF materials for gas separation across various pressures.