UNIVERSITY OF DELAWARE

CHEMICAL & BIOMOLECULAR ENGINEERING

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PHYSICS-INSPIRED MACHINE LEARNING POTENTIALS FOR THERMODYNAMIC AND DYNAMIC PROPERTIES OF ELECTROLYTE SOLUTIONS

Understanding the interactions which governs aqueous electrolyte solution properties is essential to advancements in countless domains, from electrochemistry to biochemistry. While molecular simulations have been extensively applied to study these systems, conventional empirical force fields fail to accurately predict many thermodynamic and dynamic properties, indicating limitations in capturing the underlying physics. In this talk, I will present our efforts in developing machine-learning potentials (MLPs) fit to a first-principles derived potential energy surface that can overcome these deficiencies. Moreover, we decompose energetics to identify physical underpinnings that contribute most to the property predictions. I will also describe our efforts in applying these potentials to better understand how electrolytes behave in confined environments and at hydrophobic interfaces. These studies highlight applications of machine learning for molecular simulations to not only improve property predictions but also achieve greater physical interpretability.