ABSTRACT

This dissertation advances computational frameworks for rational molecular design and modeling across multiple application domains. The work demonstrates the use of both quantum chemical and classical methods to improve predictive accuracy and gain greater mechanistic insights. In the domain of energy storage, this work proposes design rules for fluoride-ion batteries (FIBs) by integrating genetic algorithms (GA), machine learning (ML), quantum chemical (QC) calculations, and molecular dynamics (MD) methods. Additionally, investigations into solvent-driven high entropy electrolytes (HEE) through high-throughput MD reveal the fundamental limits of entropy-induced transport enhancement. To advance simulation capabilities for reactive systems, the dissertation introduces the Hybrid Kinetic Monte Carlo/Molecular Dynamics (HkMCMD) framework, offering a novel approach for simulating reactive systems. Extending these principles to broader chemical challenges, the work analyzes prebiotic reverse Tricarboxylic Acid (rTCA) reaction networks using reaction prediction methods, highlighting the dominance of kinetic accessibility over thermodynamic favorability. Finally, a study on rational design of cations for per- and polyfluoroalkyl substances (PFAS) ion-exchange (IX) resins demonstrates how electronic softness and charge delocalization can be systematically tuned to achieve improved selectivity for PFAS remediation.