ABSTRACT

This thesis investigates transport phenomena under nanoscale confinement with a focus on developing a unified, physics-driven multiscale framework that connects molecular mechanisms to system-level performance. When fluids, ions, and polymers are confined to dimensions comparable to their molecular sizes, classical continuum descriptions fail as interfacial forces, entropic constraints, electrostatic correlations, and molecular layering dominate the system response. Through molecular dynamics simulations, this work elucidates the coupled roles of confinement, wettability, surface chemistry, and soft-matter interactions in governing water, ion, polymer, and multiphase transport in nanochannels.

The thesis first establishes molecular design principles for graphene-based desalination membranes by analyzing pressure-driven flows, solute–membrane interactions, and dehydration energy barriers controlling selectivity and flux. It then demonstrates polymer-mediated control of nanofluidic interfaces, revealing how polymer orientation, grafting density, and chemistry can tune slip, flow resistance, and selective transport. Multiphase nanofluidics is subsequently explored, uncovering passive fractionation pathways for oil–water systems for oil spill applications.

To translate molecular insights to engineering scales, the thesis develops a physics-informed machine learning framework that integrates atomistic descriptors into governing transport equations, enabling rapid, interpretable predictions of system-level quantities such as desalination performance metrics. Finally, the multiscale understanding is extended to applications in thermal management and renewable energy through the design and synthesis of polyacrylamide–lithium chloride composite hydrogels. These materials are demonstrated as passive cooling solutions for electronics and photovoltaic modules, illustrating the practical scalability of the proposed framework.

Overall, this thesis advances the fundamental understanding of transport under extreme confinement, establishes nanoscale control knobs through interfacial physics and soft matter interactions, and bridges molecular simulations to real-world desalination, environmental remediation, and cooling technologies through physics-informed artificial intelligence.