ABSTRACT

With the system length scales becoming comparable to the molecular dimensions, flow of fluids through nanofluidic channels leads to several non-intuitive and interesting phenomena which are otherwise not observed at larger length scales. Water, despite not being a complex fluid as per classical hydrodynamics, has complexities associated at the molecular levels, giving rise to anomalous properties. Nature widely uses this amalgamation of the continuum properties and the molecular attributes in nanopores and membranes; hydrophobic self-cleaning leaves and scales, antifogging functionality of insect eyes, natural adhesion in gecko limbs, water transport in cells, hydrophilic leaves of pitcher plant etc. Development of manufacturing techniques and discovery of materials like carbon nanotubes and graphene have made it plausible to employ nanofluidics to laboratory and industrial applications. The precise control over fluid steering and retention, over these scales, can form the basis of several applications related to fluid transport, mixing, drug delivery and energy conversion. Through extensive molecular dynamics simulations of water in nanochannels, we develop a comprehensive theoretical understanding of the molecular phenomena and the upscale implications on its dynamics providing a blueprint for futuristic experimental studies.

The dissertation begins with the discussion of anomalous filling rates of nano-capillaries arising from the interfacial interaction, leading to a dynamic slip length along the capillary axis. The subsequent analysis discusses the effect of size and hydration properties of ionic inclusions on slip length of saline solutions and using it to tune the wettability. We further discuss the effect of gas phase in a closed end capillary with the gas compressed between the meniscus and walls alternately accelerating and retarding the filling.

The other half of the dissertation deals with electrokinetic phenomena at nanoscales. The development of surface charge and the electric double layer formation are shown to alter the slip length and the flow dynamics which affect the electrokinetic energy conversion. We further discuss the blueprint for optimizing various parameters to maximize energy conversion efficiencies in nanofluidic circuits.

Keywords: Nanofluidics, molecular dynamics, wettability, slip length, stick-slip motion, ionic inclusions, electrokinetics, electromechanical energy conversion.