ABSTRACT

Title of Dissertation:	WATER, ION, AND GRAPHENE: AN ODYSSEY THROUGH THE MOLECULAR SIMULATIONS
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Water is known as the most common and complicated liquid on earth. Meanwhile, graphene, defined as single/few layer graphite, is the first member in the 2-dimensional materials family and has emerged as a magic material. Interactions between water and graphene generate many interesting phenomena and applications. This thesis focuses on applying molecular dynamics (MD), a powerful computational tool, for investigating the graphene-water interactions associated with various energetic and environmental applications, ranging from the wettability modification, species adsorption, and nanofluidic transport to seawater desalination. A key

component of one domain of applications involves a third component, namely salt ions. This thesis attempts that and discovers a fundamentally new way in which the behavior of ions with the air-water interfaces should be probed.

In Chapter 1, we introduce the motivation and methods and the overall structure of this thesis. Chapter 2 focuses on how MD simulations connect the statistical mechanics theory with the experimental observations. Chapter 3 discusses the simulation results revealing that the spreading of a droplet on a nanopillared graphene surface is driven by a pinned contact line and bending liquid-surface dynamics. Chapter 4 probes the interactions between a water drop and a holey graphene membrane, which is prepared by removing carbon atoms in a circular shape and which can serve as catalyst carriers. Accordingly, chapter 5 studies the effects of various terminations on water-holey graphene interactions, showing that water flows faster and more thoroughly through the membrane with hydrophobic terminations, compared to that with hydrophilic terminations. In chapter 6, simulations describe the generation of enhanced water-graphene surface area during the water-holey-graphene interactions in presence of an applied time-varying force on the water drop. In chapter 7, we focus on the ion-water interaction at the water-air interface to fully understand the fluidic dynamics during any seawater desalination. Our research revisits the energetic change while ion approaches water-air interface and shows that the presence of ion at the interface enhances capillary-wave fluctuation. Finally, in chapter 8 we summarize the main findings of the thesis and provide the scope of future research.