Development of Interface Potential Based Methods for Calculating the Wetting Properties of Complex Systems

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The behavior of fluids at solid surfaces plays a significant role within numerous natural phenomena and industrial applications. To this end, understanding and predicting the interfacial properties of these systems is crucial for the development of emerging technologies. Within our group, we have developed an interface potential approach for determining interfacial properties. In previous work, we performed simulations within a grand canonical ensemble and calculated the interface potential using transition matrix Monte Carlo methods. However, there are limitations to working within this ensemble, particularly when applying the technique to complex molecules and working at relatively low temperatures. Recently, we developed a means for calculating the interface potential using an isothermal-isobaric ensemble (NPT) using molecular dynamics. In this presentation, we discuss how to implement this approach within a molecular dynamics framework. We perform simulations in the canonical ensemble at different volumes to sample states. We use the forces acting on the substrate to construct an interface potential. Expanded ensemble techniques are used to evaluate interfacial properties over a range of temperatures and surface characteristics. Molecular dynamics simulations are performed using the LAMMPS package. Results are presented for water on a silica surface and 1,3-diMethylImidazolium tetraFluoroBorate ([C1MIm]BF4) on a graphite surface. The results obtained using molecular dynamics are compared with those obtained from grand canonical Monte Carlo simulation.