

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Parameterization of Nonbonded Interactions between Molybdenum Disulfide and Water MOHAMMAD HEIRANIAN, YANBIN WU, NARAYANA ALURU, University of Illinois at Urbana-Champaign — Recently, single-layer nanoporous molybdenum disulfide (MoS_2) membranes have been found to be a promising material in various applications such as DNA sequencing, water purification and power generation. To understand the physics taking place in such nanofluidics systems, an accurate forcefield is needed to describe the van der Waals and coulombic interactions between MoS_2 and water. In this work, the high-accuracy adiabatic-connection fluctuation-dissipation based random phase approximation (RPA) method is used to implement water- MoS_2 parameters for use in molecular dynamics simulations. The accuracy of the developed parameters is validated by comparing the resulting water- MoS_2 contact angle, an interface property, from MD with that of experiments. The accurate description of water- MoS_2 interface, studied here, will facilitate the future studies of the above-mentioned applications.

Mohammad Heiranian
University of Illinois at Urbana-Champaign

Date submitted: 10 Nov 2016

Electronic form version 1.4