Abstract Submitted
for the DFD17 Meeting of
The American Physical Society

Atomistic Modeling of the Fluid-Solid Interface in Simple Fluids

NICOLAS HADJICONSTANTINOU, GERALD WANG, MIT — Fluids can exhibit pronounced structuring effects near a solid boundary, typically manifested in a layered structure that has been extensively shown to directly affect transport across the interface. We present and discuss several results from molecular-mechanical modeling and molecular-dynamics (MD) simulations aimed at characterizing the structure of the first fluid layer directly adjacent to the solid. We identify a new dimensionless group – termed the Wall number – which characterizes the degree of fluid layering, by comparing the competing effects of wall-fluid interaction and thermal energy. We find that in the layering regime, several key features of the first layer layer – including its distance from the solid, its width, and its areal density – can be described using mean-field-energy arguments, as well as asymptotic analysis of the Nernst-Planck equation. For dense fluids, the areal density and the width of the first layer can be related to the bulk fluid density using a simple scaling relation. MD simulations show that these results are broadly applicable and robust to the presence of a second confining solid boundary, different choices of wall structure and thermalization, strengths of fluid-solid interaction, and wall geometries.

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Date submitted: 31 Jul 2017 Electronic form version 1.4