Abstract Submitted
for the DFD17 Meeting of
The American Physical Society

**Layering at the Fluid-Solid Interface and Anomalous Diffusion in Nanoconfined Fluids** GERALD WANG, NICOLAS HADJICONSTANTINOU, MIT — Molecular self-diffusion in a fluid under nanoconfinement can differ considerably from its counterpart in the bulk; this "anomalous" diffusion can have profound implications for applications involving transport in nanoconfined systems. In this talk we study the contribution of fluid layering at the solid-liquid interface to anomalous diffusion, using molecular-mechanical modeling and molecular-dynamics (MD) simulations of simple fluids confined within a graphene nano-slit. We find that fluid layering near the fluid-solid interface strongly affects molecular diffusion; the former can be characterized by a non-dimensional group – referred to as the Wall number – which compares the competing effects of wall-fluid interaction and thermal energy. We specifically demonstrate that the dependence of the *overall* diffusion coefficient on the confinement lengthscale can be modeled by superposing the contributions of the bulk and near-wall regions. The anomalous diffusive behavior in the near-wall region is due to a "dimensional restriction" of the near-wall fluid. MD simulation results suggest that the difference between the bulk and near-wall diffusivity can be modeled using the excess entropy of the fluid in each region.

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Date submitted: 31 Jul 2017 Electronic form version 1.4