

Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Polystyrene films confined between gold surfaces

KAREN JOHNSTON, Max Planck Institute for Polymer Research, VAGELIS HARMANDARIS, University of Crete, KURT KREMER, Max Planck Institute for Polymer Research — The properties of thin short-chain polystyrene films between two parallel Au(111) surfaces are studied using a combination of density functional theory (DFT) and classical molecular dynamics (MD) simulations. The chemical interaction with the surface is calculated with DFT and the results are used to develop accurate atomistic classical surface potentials. These potentials are used in the MD simulations to investigate several systems with various film thickness and the effect of increasing confinement on the structural and dynamical properties of the films will be presented. A coarse-grained model is developed and used to study longer-chain polystyrene films and larger systems.

Karen Johnston
Max Planck Institute for Polymer Research

Date submitted: 05 Oct 2011

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