Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Simulations of Nanoscale Mechanical Contacts with Intervening Adsorbates[1] SHENGFENG CHENG, MARK ROBBINS, Department of Physics and Astronomy, The Johns Hopkins University, Baltimore, MD 21218 — Molecular simulations are used to investigate the role of intervening adsorbed molecules in nanometer scale mechanical contacts between nominally spherical tips and flat elastic substrates. Previous studies show that atomic scale deviations from the sphere that are present on any tip constructed from discrete atoms can have profound effects on contact areas, adhesive energies, and lateral stiffness. We find that including adsorbed molecules in contacts reduces the variation with tip geometry, but introduces new effects. One is that tip geometry affects the number of atoms that are pushed out of the contact and the resulting pressure distribution. The pressure at the center of the contact may be smaller than at the edge. We also find that the presence of adsorbates influences frictional behavior of contacts. For some cases the frictional force is proportional to area for bare tips and proportional to load when adsorbed molecules are present.

[1]This work was supported by NSF Grant DMR-0454947.

Shengfeng Cheng
Department of Physics and Astronomy
The Johns Hopkins University, Baltimore, MD 21218

Date submitted: 25 Nov 2006 Electronic form version 1.4