Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Density-functional study of adsorption of isocyanides on the gold (111) surface.[1] YULIA GILMAN, PHILIP B. ALLEN, Department of Physics and Astronomy, SUNY Stony Brook — Density functional theory (DFT) is used to study how the isocyanides HNC and CH_3NC attach to the gold (111) surface. Slab calculations are performed for monolayers with 1 molecule per 3 gold atoms coverage. For both molecules a weak binding of about 0.2 eV is found at the top site. No binding is found at other sites.

[1]This work was supported in part by NSF Grant NIRT-0304122.

Yulia Gilman
Department of Physics and Astronomy, SUNY Stony Brook

Date submitted: 03 Dec 2004 Electronic form version 1.4