Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Structural and Electronic Properties of Aromatic Isocyanide Self-Assembled Monolayers on Au(111) Surface YAN LI, GIULIA GALLI, Department of Chemistry, University of California, Davis, CA, 95616 — The search for molecular assemblies with interesting transport properties for molecular electronic devices is an active field of research. Isocyanide self-assembled monolayers (SAMs) have received some attention lately, as they may provide a better π-network for electron transport than other molecular SAMs such as benzenethiols. We have studied the structural and electronic properties of the interface between a gold surface and an aromatic isocyanide SAM, using density-functional theory in the GGA-PBE approximation. Our calculations predict a herringbone arrangement at high coverage, instead of the conventional structure with $(\sqrt{3} \times \sqrt{3})R30^\circ$ periodicity. The most favorable geometry is however found at low coverage, where the interaction between molecules is negligible and the barriers between differently tilted geometries are small compared to room temperature. These results explain the disordered patterns recently observed in room temperature STM measurements and point at possible difficulties in using isocyanide SAMs for molecular devices. Our calculations also give insight into the alignment of the molecular energy levels with respect to the Fermi energy of the metal substrate, and the charge redistribution at the interface, which provide essential guide for understanding and predicting transport properties of these SAMs, in case ordering can be achieved.

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Date submitted: 20 Nov 2006 Electronic form version 1.4