Abstract Submitted
for the NEF09 Meeting of
The American Physical Society

Modeling the Self-Assembly of Carboxylic Acid Substituted Fullerenes on Au(111) GREGORY BUBNIS, HOWARD MAYNE, University of New Hampshire — Self-assembled surface architectures incorporating functionalized fullerenes have been studied extensively; However, the prediction and rational design of molecular scale patterns remain challenging. For small organic molecules, hydrogen bonding functional groups are often used as the dominant intermolecular interaction to drive self-assembly. We focus on a family of fullerenes with carboxylic acid terminated phenyl, biphenyl, and (linear) polyphenylene substituents to study their monolayer pattern formation on Au(111). All-atom modeling efforts for such systems are often limited to small clusters and the most accurate *ab initio* calculations can require experimental guidance because exhaustive explorations of configuration space are intractable. We develop simplified potential energy functions for the relevant physical interactions and constrain the molecules and surface to be rigid. This "coarse-grained" approach permits studies of 25 to 50 molecules – using unbiased Metropolis Monte Carlo simulations to thoroughly explore the configuration space – at a modest computational expense. Fullerene moieties are found to form hexagonal monolayers and substituent groups dictate additional orientational order. The largest substituents hinder pattern formation while parallel, one-dimensional hydrogen bonded chains as well as herringbone patterns are observed in other cases.

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Date submitted: 28 Sep 2009 Electronic form version 1.4