

Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

A Model Study of Structural Phase Changes in Clusters of Derivatized Fullerenes on Au(111) GREGORY BUBNIS, HOWARD MAYNE, University of New Hampshire — Self-assembled adsorbate layers incorporating derivatized fullerenes have been studied extensively and recently reviewed. [Sánchez et al. *Chem. Rev.*, 2009, **109**, pp 2081–2091] But the prediction and rational design of their preferred structures remains challenging. We have initiated a systematic modeling study of pattern formation of derivatized fullerenes on the Au(111) surface. We focus on a family of fullerenes with carboxyl functionality capable of strong intermolecular hydrogen bonds. The carboxyl groups are bonded to the fullerene using phenyl, biphenyl, and (linear) polyphenylene linkages. The relevant intermolecular interactions are described by simplified potential energy functions and we constrain the molecules and surface to be rigid. Metropolis Monte Carlo simulations are carried out on clusters at a range of temperatures and the adlayer structure is inferred from the heat capacity as well as several structure parameters. Our coarse-grained approach permits the study of clusters as large as fifty molecules at a relatively modest computational expense. Our results show that fullerene moieties prefer to form hexagonal close-packed monolayers and the substituent groups dictate additional orientational order. Extended one-dimensional hydrogen bonded chains can be formed for bifunctional fullerenes. For monofunctional fullerenes, hydrogen bonding leads to the formation of herringbone adlayers. Furthermore, we show pure dispersion intermolecular interactions can also lead to herringbone patterns. The largest substituents hinder pattern formation.

Gregory Bubnis
University of New Hampshire

Date submitted: 20 Nov 2009

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