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Replica exchange Monte Carlo simulations of derivatized fullerenes on Au(111) HOWARD MAYNE, GREG BUBNIS, University of New Hampshire — Self-assembling surface architectures incorporating derivatized C60 fullerenes have been studied extensively. However, predicting and designing molecular scale patterns remains challenging. By using hydrogen bonding forces as the dominant intermolecular interaction, many small organic molecules can self-assemble into predictable, robust structures. With this in mind, we study pattern formation of a family of C60 fullerenes with carboxylic acid-bearing substituents on the Au(111) surface. Molecules containing two and three fullerene moieties are also considered. Our "coarse-grained" modeling approach preserves the dominant physical interactions between molecules and uses rigid constraints to reduce computational expense. With this, we carry out temperature replica exchange Metropolis Monte Carlo simulations of 25 to 50 molecules and obtain a thorough sampling of the configuration space. Averages of the energy and structural order parameters are used to measure patterning and phase changes over a range of temperatures. We also explore how patterning is influenced by varying parameters such as surface corrugation and both intermolecular and molecule-surface interaction energies.

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