Monte Carlo Study of the Honeycomb Structure of Anthraquinone Molecules on Cu(111)[1] KWANGMOO KIM, T. L. EINSTEIN, University of Maryland, College Park, LUDWIG BARTELS, University of California, Riverside — Using Monte Carlo calculations of the two-dimensional (2D) lattice gas model, we demonstrate a mechanism for the spontaneous formation of honeycomb structure of anthraquinone (AQ) molecules on a Cu(111) plane. Unlike the suggestion of long-range substrate-mediated repulsion,[2] long-range attractions play important roles in our calculations. However, the interplay between attractions and repulsions is still integral to the spontaneous formation of AQ's honeycomb structure. We also compare the critical local coverage rate of AQ's where the honeycomb structure starts to form. Furthermore, we study the diffusion of CO molecules inside AQ honeycombs on the Cu(111) plane. The surface phase transitions of CO molecules between solid, liquid, and gas 2D phases are studied via the specific heat singularity in short-range correlation functions.[3]

[2]Greg Pawin *et al.*, Science **313**, 961 (2006).
[3]N. C. Bartelt, T. L. Einstein, and L. D. Roelofs, PRB **32**, 2993 (1985).

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