Abstract Submitted
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Monte Carlo Study of the Diffusion of CO Molecules inside Anthraquinone Hexagons on Cu(111)[1] KWANGMOO KIM, T.L. EINSTEIN, Univ. Maryland, JON WYRICK, LUDWIG BARTELS, Univ. California–Riverside — Using Monte Carlo calculations of the two-dimensional (2D) lattice gas model, we study the diffusion of CO molecules inside anthraquinone (AQ) hexagons on a Cu(111) plane. We use experimentally-derived CO-CO interactions[2] and the analytic expression for the long-range surface-state- mediated interactions[3] to describe the CO-AQ interactions. We assume that the CO-CO interactions are not affected by the presence of AQ's and that the CO-AQ interactions can be controlled by varying the intra-surface-state (ISS) reflectance r and the ISS phase shift δ of the indirect-electronic adsorbate-pair interactions. Comparing our results with experimental observations, we find that not only pair but also surface-state-mediated trio interactions[4] are needed to understand the data.

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