Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Diffusion of anthracene derivatives on Cu(111) studied by STM and DFT JONATHAN WYRICK[1], LUDWIG BARTELS, University of California at Riverside, THEODORE EINSTEIN, University of Maryland — Substituted anthracenes have drawn attention due to their ability to diffuse uniaxially on a Cu(111) surface. We compare anthracene to three of its derivatives whose 9,10 hydrogens are replaced by elements of the chalcogen group that act as linkers binding the molecules to a Cu(111) substrate. DFT calculations shed light on STM imaging and diffusion studies on the three substituted species. We present an analysis of the DFT results in which energetic contributions to the diffusion barriers are partitioned among the Kohn-Sham orbitals, allowing us to make assignments as to how each orbital affects diffusion for each species and draw comparisons between them.

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Date submitted: 14 Nov 2013 Electronic form version 1.4