Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Diffusion of two-dimensional Cu islets on Ag(111) studied with the Molecular Dynamics Method SADAR S. HAYAT, The Islamia University of Bahawalpur, MARISOL ALCANTARA ORTIGOZA, TALAT S. RAHMAN, University of Central Florida — Our molecular dynamics simulations (at 300, 500 and 700 K) of the diffusion of two-dimensional Cu_n islets ($1 \leq n \leq 9$) on Ag(111) using many-body potentials yield an Arrhenius behavior. Concerted motion is seen to dominate the diffusion of smaller islets (2-4 atoms) whereas multiple-atom, shape-adjusting processes control the diffusion of the larger ones. Although the effective energy barrier scales with islet size, the barriers do not change considerably for islands containing 4 to 9 atoms (they are $\sim 220 \pm 37$ meV). While the diffusion barrier for Cu monomers on Ag(111) is higher than that on Cu(111) (both in experiment and theory), the situation reverses starting from the dimer. Our results for monomer and dimer are in excellent agreement with those extracted from experiments.[1] On comparing our results with those for Cu islets on Cu(111), we find that the comparatively large Ag-Ag bond-length sets the contrast between Cu monomer diffusion on Cu(111) and on Ag(111). The diffusivity of Cu dimer, however, is boosted on Ag(111) by the competition between optimizing the Cu-Cu and the Cu-Ag bonds. For larger islets (3-9 atoms) our results reveal several novel diffusion processes, including those in which an islet-atom climbs atop. [1]Morgenstern *et al.* PRL**93**, 056102 (2005). Work supported by NSF-ITR 0428826.

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Date submitted: 29 Nov 2008 Electronic form version 1.4