Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Adatom Diffusion on Ag(100) and Cu (100) Surface with Steps: insights from *ab initio* electronic structure calculations[1] HANDAN YILDIRIM, ABDELKADER KARA, TALAT RAHMAN, University of Central Florida, PHYSICS DEPARTMENT TEAM — We present results of calculations of the activation barriers for an adatom (Ag or Cu) diffusing on terraces of Cu(100) and Ag(100), with steps on them. Our results based on the density functional theory (DFT) with the generalized gradient approximation, present systematic differences with those obtained using semi-empirical potentials. For the Ag systems, the latter are always higher than the former by about 40 meV, except for the case of hopping over the step where it is higher by 130 meV. The opposite is the case for Cu for which lower values are obtained by semi-empirical potentials than by DFT, except for the case of hopping over the step where this value is overestimated by the semi-empirical potentials. In examining the subtleties in the differences between the Ag and Cu systems, analysis of the d-band of the adatom in the hollow and bridge site show a systematic shift of the band towards higher energies when moving from hollow to saddle points. Moreover, Ag systems show a large narrowing of the d-band as opposed to the Cu cases where it is not noticeable. For adatom diffusion on the terraces (without steps) of Ag(100) and Cu(100), our calculations are in agreement with previous results.

[1]This work was supported by NSF-ITR 0428826

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Date submitted: 02 Dec 2006 Electronic form version 1.4