Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Exploring the Role of Steps: A Collection of Case Studies of Vicinal Metal Surfaces using Density Functional Theory JAMES WESTOVER, ABDELKADER KARA, University of Central Florida — We will present results from multiple case studies done using DFT. We have explored the contribution made by step edges when metal surfaces are in contact with organic molecules, specifically, the cases involving pentacene ($C_{22}H_{14}$). The cases of vicinal surfaces with terrace geometries of 100 and 111 will be compared and contrasted. The question of terrace width is also addressed by results presented for situations involving diminishing step width. Because of the abundance of experimental data for copper it has been chosen as one metal surface to be considered. Additionally, copper's lattice constant is commensurate with the ring width in the benzene chain that forms pentacene. To contrast copper results for another noble metal, silver, will also be presented. We will present results for both structural and electronic changes in both the substrate and molecule.

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Date submitted: 09 Nov 2012 Electronic form version 1.4