Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Electronic Structure of Arenene-Transition Metal-Graphene Complexes S.C. BADESCU, NRL, Washington, DC, V.M. BERMUDEZ, D.E. BARLOW, T.L. REINECKE, NRL, Washington, DC — The interaction between the electronic structures of transition metals and pi-conjugated species leads to the formation of organometallics, of interest in particular for their catalytic properties. With the availability of high-quality graphene, new hybrid structures with controllable electronic properties become attractive for electronics. We report calculations of 'sandwich' structures containing transition metals between aromatic molecules and graphene. First we identify the adsorption geometries of metal atoms with emphasis on the minimal clustering regimes. Then we find the adsorption structures and electronic properties of aromatic molecules on the metal-graphene substrate. The adsorption of aromatics is greatly enhanced by the metal atoms due to strong hybridization between their pi-orbitals with the metal d-states. We study the ground-state electronic and magnetic properties of these systems. We also analyze their electronic excitations that can be related to spectroscopy data.

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Date submitted: 20 Nov 2009 Electronic form version 1.4