Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

An extensive computational study of the adsorption of thiophene on transition metal surfaces: role of van der Waals[1] TOMAS ROJAS, ABDELKADER KARA, Department of Physics, University of Central Florida — Van der Waals (vdWs) interactions play a significant role in the determination of the adsorption characteristics at the interface between a molecule and a substrate. In this study, self-consistent inclusion of vdW interactions in density functional theory provides a good perspective to understand the interaction between organic adsorbates and inorganic interfaces. We present the results of adsorption of thiophene (C_4H_4S) on various transition metal surfaces with the goal of comparing the performance of five different vdW functionals (optB86, optB88, optPBE, revPBE, rPW86). Seven metallic substrates (100) are used for our study; three coinage metals (Au, Ag, Cu) and four reactive metals (Pt, Pd, Rh, Ni). The results show that vdWs inclusion enhances the interaction for Ag (0.08 to 0.73 eV), Au (0.14 to 0.86 eV), Cu (0.12 eV to 0.77 eV), Ni(1.56 to 2.34 eV), Pt (1.6 to 2.51 eV), Pd (1.67 to 2.54), Rh (1.74 to 2.96 eV). In addition, we performed calculations for adsorption heights along with analysis of the electronic changes (charge transfer, changes in the d-band of the substrate, and change in the work function) to complement our understanding of these systems.

[1]This work is funded by the U.S. Department of Energy Basic Energy Science under Contract No DE-FG02-11ER16243

Abdelkader Kara
Department of Physics, University of Central Florida

Date submitted: 14 Nov 2013 Electronic form version 1.4