

Abstract Submitted  
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**Adsorption characteristics of Thiophene on Cu and Ni(100): role of van der Waals**<sup>1</sup> TOMAS ROJAS, JERONIMO MATOS, ABDELKADER KARA, Department of Physics, University of Central Florida — We apply density functional theory, with and without the inclusion of self-consistent van der Waals (vdWs) interactions (optB86, optB88, optPBE, revPBE, rPW86), to study the adsorption of thiophene (C<sub>4</sub>H<sub>4</sub>S) on Cu(100) and Ni(100). Our calculations reveal that the C<sub>4</sub>H<sub>4</sub>S molecule adsorbs, on either substrate, with its molecular plane parallel to the surface with the sulfur close to the bridge site. The inclusion of vdWs interactions results in a significant increase in the binding energy of thiophene on Cu(100) (from 0.12 eV to up to 0.77 eV), while the adsorption height is also modified from 3.2 Å down to, at most, 2.38 Å, depending on the functional used. The Ni(100) case presents a similar behavior for the binding energy (enhancement from 1.56 eV to up to 2.34 eV), but the adsorption heights increase from 2.12 Å up to 2.32 Å. In addition to adsorption geometry and energetics, we present the results and analysis of the electronic properties (charge transfer, changes in the d-band of the substrate, and change in the work function) of these two systems to complement our understanding of the molecule-substrate bonding. Our results suggest that the adsorption characteristics are dependent on the type of functional used; opt-type functionals (optB86, optB88, optPBE) are found to produce stronger bonding as compared to PBE, revPBE and rPW86.

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