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**Adsorption of thiophene on Pt, Pd, Au, and Rh(100) surfaces with the role of the van der Waals' interaction** WALTER MALONE, JERONIMO MATOS, ABDELKADER KARA, University of Central Florida — We explore the adsorption of thiophene (C<sub>4</sub>H<sub>4</sub>S) on Pt(100), Au(100), Pd(100), and Rh(100) surfaces using density functional theory with and without self-consistent van der Waals interactions (vdWs). The six functionals we use are PBE, optB86b-vdW, optB88-vdW, optPBE-vdW, revPBE-vdW, and rPW86-vdW2. We examine a variety of adsorption sites with the molecule's plane both parallel and perpendicular to the surface. In the case of parallel adsorption the highest binding energy occurs when the molecule is centered over a hollow site with the sulfur atom near an atop site. The highest adsorption energy for perpendicular configurations is achieved when the sulfur atom lies over a bridge site and the carbon atoms near hollow sites. We find that for thiophene on the coinage metals the vdW functionals predict higher adsorption energies than those predicted by the PBE functional. On the other hand, for thiophene on the reactive transition metal substrates only optB86b-vdW, optB88-vdW, and optPBE-vdW result in an enhancement in the adsorption energy over the PBE value. We also explore some of the electronic properties of the system including charge transfer and change in the work function. Our results indicate that adsorption characteristics depends heavily on the functional used and geometry.

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