

Abstract Submitted  
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**Adsorption of thiophene derivatives on gold: an experimental and theoretical investigation** WALTER MALONE, University of Central Florida, TINGMING JIANG, YONGFENG TONG, University of Paris-Saclay, DIANA DRAGOE, University of Paris-Sud , AZZEDINE BENDOUNAN, University of Paris-Saclay, ABDELKADER KARA, University of Central Florida, VLADIMIR ESAULOV, University of Paris-Saclay — We investigate using Density Functional Theory (DFT) and Core Level measurements the adsorption of several thiophene derivatives including thiophene( $C_4H_4S$ ), bithiophene ( $C_6H_6S$ ), and terthiophene ( $C_{12}H_8S$ ) on an Au(111) surface. Specifically, we look at the change in the  $2p$  core level of the sulfur, and any geometric changes that may occur upon adsorption. We explore several adsorption configurations with the plane of the molecule perpendicular or parallel to the surface. We also investigated the possibility of broken C-S bond and its implications on the adsorption characteristics. The calculations were performed using the Vienna Ab initio Simulation Package (VASP) using a van der Waals force inclusive (vdW) functional, optB88-vdW. The XPS and NEX-AFS experiments were done at the French synchrotron SOLEIL and on an in-house high resolution XPS setup on both Au(111) crystal surface and on gold on mica substrates. Comparisons between experimental and computational results will be presented.

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