

Abstract Submitted
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The impact of functional group on the electronic structure of coordination center¹ ZAHRA HOOSHMAND GHAREHBAGH, DUY L, TALAT S RAHMAN, University of Central Florida — While 9, 10 dicyano-anthracene (DCA) forms a coordination network on Cu(111) surface with Cu adatom coordinated by three DCA molecules [1], its isomers, 9,10-diisocyano-anthracene forms, surprisingly, molecular rows on the same surface [2]. To understand the impact of functional groups on the electronic structure of the coordination center, we have carried out density functional theory based calculations of the electronic structure of a set of naphthalene molecules with different functional groups (N, CN, NC, NH₂, COH, COOH) adsorbed on Cu(111), with and without a Cu adatom. Our results show that while the interaction between the naphthalene backbone and the Cu(111) surface is dominated by van der Waals (vdW) forces, in all cases considered the functional group forms a covalent bond with the Cu (ad)atom (on) of the surface. The calculated differential charge redistribution shows that the strongest covalent bond is formed by the NC group, which differs remarkably from that formed by the CN group, while the vdW interaction is very similar in both cases. These results provide insights into the different surface coordination behavior of molecules with above-mentioned functional groups. 1. Pawin, G., et al., A Surface Coordination Network Based on Substrate-Derived Metal Adatoms with Local Charge Excess. *Angewandte Chemie International Edition*, 2008. 47(44): p. 8442-8445. 2. L. Bartels, Private communication.

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