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Experimental and Computational Comparison of the Self-Assembled Nanostructures of Pentacene Derivatives on Gold AMANDA LARSON, RYAN MILLER, JUN WANG[1], KARSTEN POHL, University of New Hampshire — Pentacene derivatives can tailor the standard pentacene molecule for unique properties beneficial to organic photovoltaic devices. Increased solubility, photo-oxidative resistance, thermal stability and tailor-able HOMO-LUMO gaps make novel pentacene derivatives enticing for further study. Scanning tunneling microscopy and density functional theory was used to examine the atomic interface between gold and the pentacene derivatives: 6,13-dichloropentacene (DCP) and 5,6,7-trithiapentacene-13-one (TTPO), electron donors exhibiting self-assembled monolayer structures on gold surfaces. Comparing DCP, TTPO and pentacene highlights the effects of differing substituents to the self-assembled structures. In particular, the unique 3-dimensional angular assembly of TTPO is examined and clarified through use of extensive computation. The lateral arrangement of the molecule is unique, causing the thiol substituent side of the molecule to be angled down towards the gold surface, while the long-axis of TTPO is parallel to the gold surface; distinctive from previously observed pentacene and pentacene derivative assemblies. By understanding the differences in self-assembly of similar molecules, we are developing novel pathways towards molecular control of organic-metal interfaces.

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