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The self-assembly of 5,6,7-trithiapentacene-13-one molecules on gold: from low-coverage molecular chains to monolayer coverage
AMANDA LARSON, JIAN-MING TANG, KARSTEN POHL, University of New Hampshire — Understanding electronic devices down to the atomic scale is essential for the development of novel organic molecule based nanotechnologies. 5,6,7-trithiapentacene-13-one (TTPO) is a promising organic semiconductor with potential applications in high temperature photovoltaic devices. Scanning tunneling microscopy (STM) of TTPO on the close-packed stepped Au (788) surface reveals interesting nanoscale surface structures ranging from molecular chains at low coverage to an ordered self-assembled monolayer. Density functional theory (DFT) calculations have been used to further probe this unique 3-D angular assembly, where the long-axis of TTPO is parallel to the gold surface, distinctive from previously observed pentacene and pentacene derivative assemblies on surfaces. It is the lateral arrangement of the underlying pentacene backbone of the molecule that is unique, causing the thiol substituent side of the molecule to be angled down towards the gold surface, with the oxygen angled away. Combining imaging with density functional theory calculations allows for classification of these self-assembled structures with particular interest being directed toward the interaction between TTPO and gold at this organic-metallic interface. Understanding of the structure of such interfaces can potentially guide nanoscale modifications for improved electrical transport and energy-conversion efficiency in future devices.

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