Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

STM and DFT examination of self-assembled 5,6,7-trithiapentacene-13-one on vicinal gold (788)[1] AMANDA LARSON, JEREMIAH VAN BAREN, JEREMY KINTIGH, JUN WANG, JIAN MING TANG, GLEN P. MILLER, KARSTEN POHL, University of New Hampshire — The novel pentacene derivative 5,6,7-trithiapentacene-13-one (TTPO) is a robust electron donor candidate for use in high temperature photovoltaic devices. STM imaging has revealed interesting nanoscale surface structures of TTPO molecular chains as well as an ordered self-assembled monolayer on 3.9nm wide gold (788) surface terraces. TTPO is a polar species of pentacene with centered oxygen and sulfur bridge substituents. It is along this sulfur bridge that TTPO arranges itself laterally with a small cant angle between the molecule and the gold surface. This lateral assembly varies from the common flat-lying and standing-up phases of pentacene on surfaces. 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 the structure of organic-metal interfaces with molecular precision potentially allows for the tailoring of those interfaces in order to maximize charge carrier transport.

[1]Supported by NSF-NSE Center for High-rate Nanomanufacturing

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Date submitted: 15 Nov 2013 Electronic form version 1.4