Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

High-Performance Simulations of the Diffusion Characteristics of a Pentacene Derivative on Gold Surfaces RYAN MILLER, AMANDA LARSON, KARSTEN POHL, Univ of New Hampshire — Pentacene serves as a backbone for several molecules that provide attractive qualities for organic photovoltaic devices. One of these pentacene derivatives is 5 6,7-trithiapentacene-13-one (TTPO), which is unique in that it achieves its lowest energy configuration on Au(1 1 1) surfaces with the thiol group angled down towards the surface, allowing many molecules to pack closely together and form molecular nanowires. However, TTPO diffuses on flat surfaces, making it difficult for the self-assembly process to be initiated. With the help of the low-energy sites in surface defects and Au(7 8 8) step edges, TTPO molecules can be anchored in place on surfaces, allowing for chain formation to begin. By using high-performance Density Functional Theory based molecular dynamics calculations, the molecules can be shown to stay localized to these bonding sites and serve as a basis for chain formation. In addition, by simulating various temperatures with a Nose-Hoover thermostat, we can analyze how temperature affects anchoring ability and diffusion properties.

Ryan Miller
Univ of New Hampshire

Date submitted: 09 Nov 2015 Electronic form version 1.4