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Conductance switching in organic monolayers LUIS AGAPITO, Physics Dept. and Quantum Theory Project - University of Florida, SABRI ALKIS, JEFFREY KRAUSE, Chemistry Dept., HAI-PING CHENG, Physics Dept. — Self-assembled monolayers of some organic molecules, such as the bipyridyl-dinitro (BPDN) [1], present conductance switching (toggling between ON and OFF states). The switching happens upon crossing fixed threshold values in the applied bias voltage and the device can "remember" its previous state; thus, they have potential value as electronic memory devices. We use density-functional theory to elucidate the atomistic origins of this phenomenon. Extensive geometry relaxations revealed two adsorption states; namely, an atop and a hollow adsorption geometry. The electronic structure of both adsorption states were further recalculated using localized basis functions and the electrical currents through these devices were estimated within the Landauer approximation. The atop state shows a higher current than the hollow state, which matches the ON and OFF conductance states observed experimentally. We attribute the conductance switching to fluctuations in the adsorption geometry of the monolayers. Ab initio calculations can help us to understand the atomistic causes of the memory effect, which is essential for having a systematic approach to theory-guided molecular synthesis. Supported by DOE grant DE-FG02-02ER45995.
[1] A. S. Blum, et al., Nature Materials 4, 167 (2005).

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