Electronic transport through a light-driven azobenzene molecule switch: A revisit by density functional theory study

YAN WANG, HAI-PING CHENG, Dept. of Physics and QTP, University of Florida, USA — Azobenzene, a molecule that changes conformation between trans and cis configurations, is a candidate light-driven molecule switch. Recent experiments showed that the “on” state with larger measured conductance is associated with the cis isomer, which is in contrast with our previous theoretical prediction. Here we reconsider the issue of the molecule-electrode and electrode-electrode coupling by performing a first-principles study of the electronic structures and transport properties of Au-azobenzene-Au molecule junctions. Specifically, we investigate the dependence of the conductance and the current-voltage characteristics in two types of Au electrode, 2-D Au(111) surface and 1-D Au STM tip. We find that, not only the trans to cis transformation of the molecule, but also the electrode-electrode coupling plays a critical role in determining the conductance near the Fermi level.

1Supported by US/DOE/BES/DE-FG02-02ER45995.

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Date submitted: 10 Nov 2011