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**Electronic transport through a light-driven azobenzene molecule switch: A revisit by density functional theory study**[1]

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.

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