Optimizing Transport Properties of a Potential Molecular Electronic Device

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Abstract

Future generations of electronic devices will have the dimensions of molecular size. The ability to control the transport properties of single molecules will have a major impact on this promising technology. The azobenzene molecule has been proposed recently as a component of a light-driven molecular switch. This molecule has two stable conformations in its ground state: *cis* and *trans*. The molecule can be converted from one configuration to the other by photo-excitation. Previous calculations showed that the *trans* configuration has a considerably higher conductance than the *cis* configuration. In this work, we study the effects of chemical substituents on the electron transport properties of azobenzene. The effects of such substituents are crucial in predicting structures that may have optimized properties with slightly different chemical structures. For the azobenzene studies, we include electron donating groups (-NH_2) and electron withdrawing groups (-NO_2) in meta- and -ortho positions with respect the azo group. We use aluminum nano-wires as leads and connect the molecule via -CH_2SH linkers to function as an electronic device. The transport properties are calculated using first principles methods that combine non-equilibrium Green's function (NEGF) technique with density functional theory (DFT).