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Effect of Geometry and Electronic Structure on Current Switching in Organic Molecules SHASHI KARNA, GOVIND MALLICK, US Army Research Laboratory — Unlike in the bulk inorganic semiconductor, electron transport in organic molecules exhibit strong dependence on the details of molecular geometry, nature of chemical bonds, and the electronic structure. The dependence of electron transport in organics also offers new mechanisms for current switching, not possible in bulk-inorganic semiconductors. In order to further understand and potentially utilize the molecular mechanisms of current switching in organic molecules, we have investigated the effect of molecular geometry, especially the change in the dihedral angle, on electron transport and current-voltage characteristics of tolane molecule with the use of *ab initio* Hartree-Fock (HF), density functional theory, and tight-binding methods within non-equilibrium Green's function approximation. The calculated results obtained from three quantum mechanical approaches vary substantially from each other. The *ab initio* HF calculations yield a maximum value for the current in the planar geometry of the molecule and minimum when the two phenyl rings are aligned perpendicular to each other.

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