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**Length and Structure Dependence of Electron Transport in Organic Molecules** SHASHI KARNA, GOVIND MALLICK, US Army Research Laboratory, HAIYING HE, RAVINDRA PANDEY, Michigan Tech University — The electron transport through organic molecules are affected by a number of structural parameters, such as the length, dihedral angle, rotation around a single-bond, symmetry and charge distribution of frontier molecular orbitals. In addition, in a molecule-solid hybrid system, the chemistry and physics of the molecule-solid interface plays an extremely important role on electron transport through organic molecules. In order to gain an enhanced understanding of the effects of length, geometry and solid-molecule interface we have investigated electron transport through  $\pi$ -conjugated molecules of increasing lengths in contact with Au substrate by non-equilibrium Green's function method within *ab initio* molecular orbital theory, density functional theory and semi-empirical methods. The effects of rotation around a single bond, change in dihedral angle and the length of the molecule on the transport properties are investigated. The results suggest a complex dependence of electron transport on one-electron energy levels, spatial characteristics of the wave function and geometry of the molecules. Further, the local density of states and location of metal Fermi level are also found to affect electron transport characteristics in a metal-molecule hybrid system.

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