APPLICATION OF DENSITY FUNCTIONAL THEORY TO PROBLEMS OF MOLECULAR ELECTRONICS

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Typically, a molecular electronic device (MED) consists of a molecule attached to two metal contacts. A key property of MEDs is their electrical conductance. The basic concepts governing current transport through molecules will be explained. We present different methods for the calculation of the conductance of MEDs that are derived from density functional theory. Various applications of our theoretical tools are discussed that aim at understanding the mechanism of electron transport. The systems studied include a molecular photo switch and polycyclic aromatic molecules.