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Molecular and Nano Scale Device-conductance: steady state and dynamical analysis

BARRY D. DUNIETZ, Univesrity of Michigan

A computational approach is used and developed to study electron transport through molecular and nano scale devices. New models and methods are employed to describe the dynamics of electron transport under the influence of time dependent (TD) perturbations. Quantum interferences affecting the TD conductance are analyzed for transient aspects, effects of present bound states and transport under the effect of coherent excitations. I will also discuss our modeling of several recent high-profile experimental studies achieving molecular scale (steady state) conductance which provides intriguing insight at the molecular structural level on the functionality of the conducting devices. The studies involve metal recognition properties of short peptides or fabricated molecular sockets based on surface confined terpyridine ligands. If time permits I will describe the required structural features for a gating field to tune the conductance of a molecular conjugated system.