# Molecular Conductance: Modeling physical and chemical control

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A model two state system is used for driving negatively the current by photo excitations. The electronic equations of motion are solved by Keldysh formalism by a simplified time-dependent perturbation theory (TD-PT) expansion.

(i)
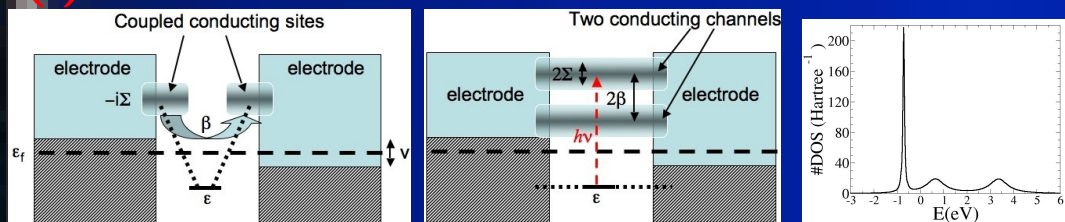
(i) Energy diagram of two-states molecular system, where only a third semi-bound lower state is fully populated at equilibrium. (right) The total electronic density of states.

(ii)
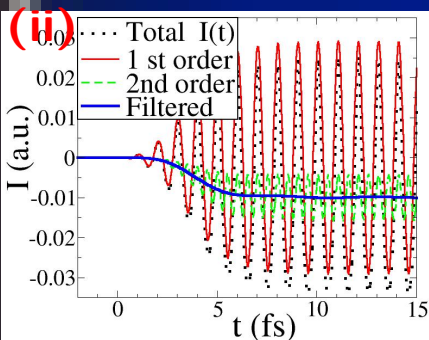
(ii) Time dependent current under weak DC bias and an AC field tuned to couple the ground and the second excited states. The first order in the TD-PT is the coherence and is fully symmetric, the second order leads to the negative current.
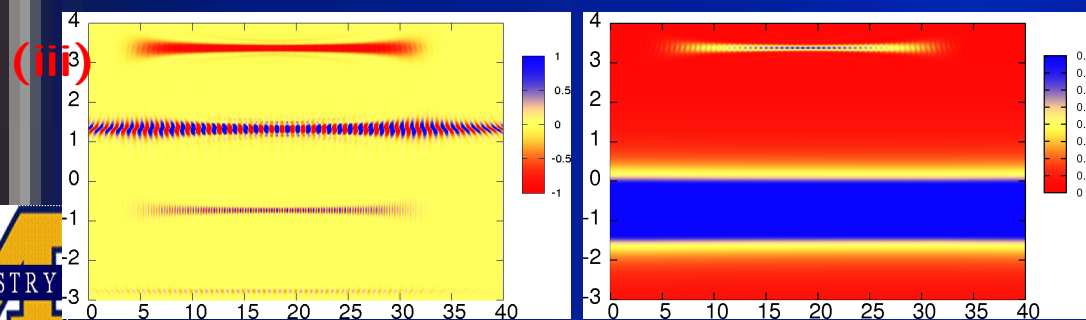
(iii) Color map of TD distribution of the (left) current operator and (right) density population. The negative current component is shown to be related to the induced population inversion where the second excited state becomes populated.

(iii)