TRANSPORT THROUGH SINGLE MOLECULE TRANSISTORS - BEYOND THE SEQUENTIAL TUNNELING AND BORN-OPPENHEIMER APPROXIMATION

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We present transport calculations for single molecule transistors using the real-time diagrammatic approach.
For complex models where the pseudo-Jahn-Teller effect forces a breakdown of the Born-Oppenheimer approximation, we present novel transport signatures of this breakdown in the sequential tunneling regime.
This occurs typically in transition metal-complexes where a local molecular shape distortions due to excess electrons competes with intramolecular tunneling of these electrons.
We show that for magnetic transition metal ions a complex interplay of spin and vibrations is possible resulting in a novel vibration-induced spin-blockade of transport.
For more simple molecular models with localized vibrational modes we address complex transport processes in the experimentally relevant regime of intermediate tunneling coupling between molecule and electrodes where sequential tunneling breaks down.
We show that novel non-equilibrium current peaks in the Coulomb blockade regime provide information on the electron-vibration coupling as well as the mechanical relaxation rate.