Kinetics of current formation in nanomolecular devices

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Recent investigation of conductive properties of nanomolecular devices (nanoleads + organic molecule) shows a strongly specific behavior of their nonlinear current-voltage characteristics including a rectification and Coulomb blockade. It has been recently revealed that such a nonlinearity is generally dictated by a molecular recharge which appears during an electron/hole transmission through the molecule. Since the recharge is connected with real occupation of the molecule by extra electrons coming from the adjacent nanoleads, a formation of the current is completely controlled by kinetic processes within the device. Based on the nonequilibrium density matrix method and using the Bogolyubov's approach for decoupling of the many-particle distribution functions, a closed set of kinetic equations for the state occupancies of the device is derived along with respective charge transfer rates. Kinetic equations have been employed to analyze an evolution behavior of the current in nanomolecular device with a single frontier molecular orbital. It has been shown that just after a sudden alteration of an applied bias voltage, the giant switch-on and switch-off currents can be formed in the device if only a coupling of the molecule to the leads differ strongly from one another. Just this circumstance is responsible for a rectification effect in the device. Both a switch-on/off effect and a rectification effect are especially pronounced at a resonant regime of charge transmission through the molecule when the capture of transferred electrons by a molecule occurs with a high probability. It is important to underline that in a nanomolecular device, a charge hopping kinetic process controls the formation not only a nonelastic component of the current but a tunnel current component as well. If more then one extra electrons occupy a nanomolecule, then due to repulsion between the extra electrons a current through the nanomolecular device can be blocked (Coulomb blockade).