Polaronic transport through molecular quantum dots: charging-induced NDR and rectification

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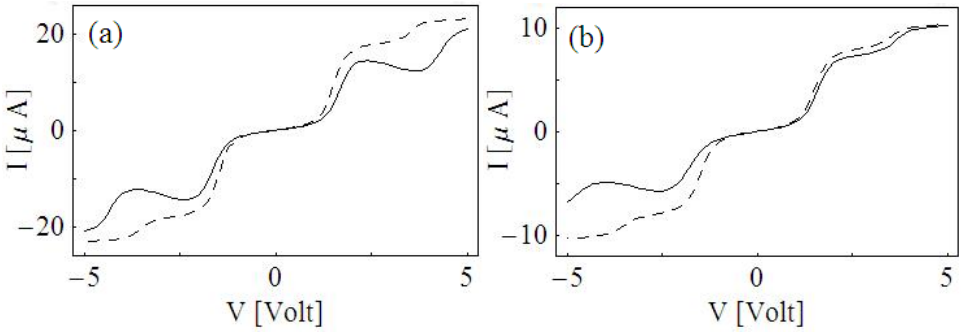
Here we study the polaronic transport through molecules weakly connected to metallic electrodes in the nonlinear response regime. Molecule itself is treated as a quantum dot with discrete energy levels, its connection to the electrodes is described within the wide-band approximation, while the charging is incorporated by means of the self-consistent potential. Nonperturbative computational scheme, used in this work, is based on the Green's function theory within the framework of polaron transformation (GFT-PT) [1]. This method transforms the many-body electron-phonon interaction problem into a one-body multi-channel single-electron scattering problem with occupation of polaron levels calculated in a self-consistent way. In particular, three different phenomena as a result of charging in polaronic transport *via* discrete quantum states are discussed in detail: the suppression of the current at higher voltages, negative differential resistance (NDR effect), and rectification.



Current-voltage (I-V) characteristics for molecular quantum dots symmetrically (a) and asymmetrically connected with two reservoirs (b) for two different charging parameters: U = 0 (dashed lines) and U = 2 (solid lines).

[1] K. Walczak, J. Magn. Magn. Mater. (2006) and Physica E (2006), both in press.

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