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Inelastic electron transport: IETS, NDR, switching, and hysteresis MICHAEL GALPERIN, Department of Chemistry, Northwestern University, ABRAHAM NITZAN, School of Chemistry, Tel Aviv University, MARK RATNER, Department of Chemistry, Northwestern University — We study the effect of the mutual influence between the phonon and the electron subsystems using nonequilibrium Green function (NEGF) formalism at the level of self-consistent Born approximation. Regarding the inelastic spectrum, two types of inelastic contributions are discussed. Features associated with real and virtual energy transfer to phonons are usually observed in the second derivative of the current I with respect to the voltage V. Signatures of resonant tunneling driven by an intermediate molecular ion appear as peaks in the first derivative dI/dV and may show phonon sidebands. The dependence of the observed vibrationally induced lineshapes on the junction characteristics, and the linewidths associated with these features are also discussed. Polaron formation on a molecular wire as a possible mechanism for observed NDR, switching and/or hysteresis in the I/V characteristic of molecular junctions is discussed within a simple mean-field model (self-consistent Hartree approximation). This mechanism differs from earlier proposed mechanisms of charging and conformational change. The polaron model captures the essential physics and provides qualitative correspondence with experimental data. The importance of active redox centers in the molecule is indicated.

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