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Understanding Nonequilibrium and Correlated Electron Behavior in Molecular Junctions

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I present an overview of the effects of the strong correlations in single-molecule junctions on non-linear transport, focusing on theory while comparing with several recent experiments. In the brief introduction I outline our real-time diagrammatic transport theory and its renormalization group extensions. In this approach a kinetic equation (generalized master equation) for the molecular density matrix incorporates both the quantum coherence and the strong correlations between electronic, vibrational and spin degrees of freedom of the device. The molecular state and non-linear current are calculated perturbatively beyond the lowest order in the coupling to the electrodes. As a first example, a detailed comparison with recent measurements on carbon-nanotube "peapod" devices is presented, indicating non-trivial hybridization and Coulomb interaction with the host nanotube quantum dot. The remainder of the talk focuses on predictions for specific electromechanical (electron-vibration coupling) and magnetic effects (spin-orbit coupling). I discuss non-linear transport signatures of vibrations when going beyond the simplified pictures of sequential tunneling (which breaks down due to quantum fluctuations) and the Born-Oppenheimer separation (its breakdown resulting in pseudo-Jahn-Teller coupling). Both effects have recently been observed. Finally, I address the interplay of transport with various aspects of molecular magnetism, such as antisymmetric (Dzyaloshinskii-Moriya) exchange and magnetic anisotropy. A comparison with recent transport experiments reveals the possibility of electric-field tunable molecular magnetism in an "ferric-star" molecular device.