MAR09-2008-002188

Abstract for an Invited Paper
for the MAR09 Meeting of
the American Physical Society

**Vibronic effects in single molecule conductance**[1]

MICHAEL THOSS, Department of Chemistry, Technical University of Munich

Recent experimental advances have allowed to study the conductance properties of single-molecule junctions and revealed a wealth of intriguing transport phenomena. An important aspect that distinguishes nanoscale molecular conductors from mesoscopic devices is the influence of the nuclear degrees of freedom of the molecular bridge. Due to the small size of molecules, the charging of the molecular bridge is often accompanied by significant changes of the nuclear geometry that indicate strong coupling between electronic and nuclear (in particular vibrational) degrees of freedom. In this contribution, the effect of electron-vibrational (vibronic) coupling on the transport properties of single molecule junctions is studied. The study is based on a combination of first-principles electronic structure calculations to characterize the system and different transport methods including inelastic scattering theory, master equations and nonequilibrium Green's function theory. The basic mechanisms of vibrationally coupled electron transport are analyzed for a generic model of a molecular junction as well as benzenealkanethiolates between gold electrodes. The results show that vibronic coupling can have a significant effect on the conductance of molecular junctions. It manifests itself in pronounced structures in the current-voltage characteristics. Moreover, the current-induced excitation of vibrational modes mays result in a significant deviation of the vibrational degrees of freedom from their equilibrium distribution.

[1]In collaboration with R. Haertle, C. Benesch, and M. Cizek, supported by the DFG and GIF