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Probing single molecule vibrations with the inelastic resonant tunneling

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Inelastic electron tunneling spectroscopy (IETS) has proven to be a valuable and powerful technique allowing identification and analysis of single molecular vibrations including those inaccessible by traditional optics measurements such as Raman and IR spectroscopies. Combined with scanning tunneling microscopy (STM) it provides a single molecule resolution. However, a comprehensive theoretical description of the electron coupling with molecular vibrations and the role it plays in conductance still remain a challenging problem. In this talk we present the first principles theory of the inelastic electron tunneling spectroscopy. Our method is based on density functional theory within Keldysh nonequilibrium Green's function formalism and allows us to treat electrons and molecular vibrations (phonons) on equal footing while computing electronic and vibrational spectrum, electron-phonon coupling, elastic and inelastic current in molecular electronic devices. The salient feature of our theory is that phonon effects on the electronic Hamiltonian are included in a self-consistent manner. Using this approach we investigate the effect of molecular vibrations on quantum transport through a C60 molecule contacted by two metallic electrodes. We demonstrate that its transport properties undergo significant changes when molecular vibrations are taken into account and show that this effect mostly originates from the resonance nature of the quantum tunneling which is expected to be true for the vast majority of the metallic electrodes. We also report a vibrational spectroscopy analysis and report those vibrational modes that contribute most to the inelastic quantum tunneling.