Theory of inelastic electron tunneling spectroscopy for probing correlated many-body systems

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We present an extension of the tunneling theory for scanning tunneling microcopy to include different types of vibrational-electronic couplings responsible for inelastic contributions to the tunnel current in the strong-coupling limit. It allows for a better understanding of more complex scanning tunneling spectra of molecules on a metallic substrate in separating elastic and inelastic contributions. The starting point is the exact solution of the spectral functions for the electronic active local orbitals in the absence of the scanning tunneling microcopy tip. This includes electron-phonon coupling in the coupled systemcomprising the molecule and the substrate to arbitrary order including the anti-adiabatic strong coupling regime as well as the Kondo effect on a free electron spin of the molecule. The tunneling current is derived in second order of the tunneling matrix element which is expanded in powers of the relevant vibrational displacements. We use the results of an ab-initio calculation for the single-particle electronic properties as a adapted material specific input for a numerical renormalization group approach for accurately determining the electronic properties of a NTCDA molecule on Ag(111) as a challenging sample system for our theory. Our analysis shows that the mismatch between the ab-initio many-body calculation of the tunnel current in the absence of any electron-phonon coupling to the experiment scanning tunneling spectra can be resolved by including two mechanisms: (i) a strong unconventional Holstein term on the local substrate orbital leads to reduction of the Kondo temperature and (ii) a different electron-vibrational coupling to the tunneling matrix element is responsible for inelastic steps in the dI/dV curve at finite frequencies.