A Priori Method for Propensity Rules for Inelastic Electron Tunneling Spectroscopy of Single-Molecule Conduction

Abstract:
An a priori computational method for determining intensities in inelastic electron tunneling spectroscopy (IETS) is developed that allows simple, chemically intuitive propensity rules to be obtained for arbitrary applications. The molecule is shown to scatter charges between quite specific eigenchannels of lead-coupling-weighted molecular density of states. This allows mode-specific scattering sites to be identified within the molecule, indicating how external chemical or other perturbations could be used to control IETS intensities.

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