

Abstract Submitted
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Modeling the Inelastic Electron Tunneling Spectra of Molecular Wire Junctions ALESSANDRO TROISI, MARK RATNER — A method to predict inelastic electron tunneling (IET) spectra through molecular junctions is proposed. The quality, reproducibility and richness of information that these measurements provide suggest that this technique could be soon become a standard way to characterize molecular junctions. However, the information contained in a IET spectrum can be useful only in the presence of a predictive model that allows its univocal assignment. Standard quantum chemical techniques are adapted to compute the Green's function derivatives with respect to the normal vibrational coordinates, and these quantities are used to calculate the intensities of the IET peak for each vibration. The agreement between the computed spectra and the experimental measurements for three different molecules recently presented by Kushmerick *et al.* [Nanoletters 4, 639, 2004] is excellent. The possibility of assigning easily an IET spectrum increases the usefulness of the technique, which, in principle can be used for *all* molecular junctions.

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