

# Theory of Single Molecule Vibrational Spectroscopy and Microscopy

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## Abstract

A recent breakthrough in Surface Science has been the experiments demonstrating vibrational spectroscopy and microscopy of single molecules by inelastic electron tunneling using a scanning tunneling microscope<sup>1</sup>. Based on density functional theory and a many-body generalization of Tersoff-Hamann theory, we have developed a theory and calculational method for this new spectroscopy<sup>2</sup>. We apply our theory to acetylene on copper and explain why only the carbon-hydrogen stretch modes are observed in terms of elastic and inelastic contributions to the tunneling conductance. The calculated values for the changes in tunneling conductance induced by these stretch modes and their spatial images are in good agreement with experiments. We find that the symmetry of the adsorbate-induced states makes the inelastic signal for the anti-symmetric stretch mode to dominate over the signal for the symmetric one. This result is in agreement with experiment and shows that the symmetries of the lowest unoccupied molecular states has an important influence on the spatial dependence of the vibrationally inelastic tunneling<sup>3</sup>.

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<sup>1</sup>B. C. Stipe, M.A. Rezaei, and W. Ho, *Science* **280**, 1732 (1998); *Physics Today* Feb. 2000, p. 17

<sup>2</sup>N. Lorente and M. Persson, (submitted to *Phys. Rev. Lett.*).

<sup>3</sup>N. Lorente, M. Persson, L. J. Lauhon, and W. Ho, (to be submitted).