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Vibrationally induced two-level systems in single molecule junctions ROBERT THIJSSSEN, Leiden University, DARKO DJUKIC, SANDER OTTE, ROLF BREMMER, JAN VAN RUITENBEEK, KAMERLINGH ONNES LABORATORY TEAM — It is found that differential conductance spectra of small single molecules contacted by metal electrodes display positive or negative peaks. The positions in energy of these peaks correspond with the energies of local vibration modes of the molecule in the junction. A model of vibrationally induced two-level systems is made in order to explain the physics responsible for the observed features. A molecule in an atomic junction can be contacted in two geometrically different configurations, each of which results into a different junction conductance. These two energy minima are separated by a large energy barrier. Only by vibrationally exciting the molecule above the barrier, a transition between the configurations is possible. This results in a sudden jump in conductance and a peak in differential conductance. The vibrationally induced two-level switching is expected to be quite general, since we have observed dI/dV peaks in many different single molecule-metal junctions. It acts as an intrinsic amplification mechanism for local vibration mode features, even when large conductance fluctuations are present. Therefore it could be exploited as a new spectroscopic tool for identifying local vibration mode energies.

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