Huge negative differential conductance in molecular nanojunctions

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The study of molecular nanojunctions built form simple molecules has attracted wide interest in the recent years [1]. The behaviour of some simple molecules bridging atomic-sized metallic junctions can already be understood in great detail mainly due to the detection of the vibrational modes with point-contact spectroscopy providing a fingerprint of the molecule. These studies are complemented by number of conductance channels analysis with conductance fluctuation and shot-noise measurements, and the quantitative predictive power of computer simulations. The above methods were successfully used to describe platinum-hydrogen junctions [2-3], it was shown that a molecular hydrogen bridge with a single, perfectly transmitting channel is formed between the platinum electrodes. For a wide variety of junctions with different electrode material and molecule however, the direct measurement of the vibrational modes fails due to the appearance of peak-like structures in the differential conductance curves [4]. We show that molecular nanojunctions can even show huge negative differential conductance. This phenomenon is found not to be a unique feature of a special atomic configuration, but it is frequently occurring in a wide conductance range and with almost all the studied molecules and contact materials, which implies the presence of a general physical phenomenon producing a similar feature under a wide range of experimental conditions. We present a detailed analysis of the observations in terms of two-level system models, demonstrating the failure of a simple TLS model [5] and the necessary ingredients for producing peak-like structures instead of simple conductance steps. A model based on an asymmetrically coupled two-level system is proposed, which can describe the observations. The comparison of the model with experimental data implies a huge asymmetry in the coupling strength, which can be explained with the physical picture of a molecule strongly bound to the junction being ”kicked out” to a large number of energetically similar loosely bound states. The proposed model grabs a feature that can lead to peak-like structures or even negative differential conductance in the dI/dV curves of molecular nanojunctions under a wide range of conditions.

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