Towards mechanical stabilization of molecular tunneling devices: Cooling by heating, high voltage, and more

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The promise for future realization of single molecule-based electronic devices relies, to a large extent, on the ability to mechanically stabilize the molecular bonds, while making use of efficient resonant charge transport through the molecules. In single molecule junctions, resonant charge transport involves excessive charging of the molecule (transiently, at least). For most organic molecules this is likely to lead to vibrational heating, conformation changes or bond rupture, which hinder the mechanical stability of the junction. Accounting for vibronic coupling during resonant charge transport is therefore essential for the realization of single molecule devices. In the talk we shall discuss several mechanisms for transport induced mechanical instability in molecular junction, and focus in particular on vibrational heating due to inelastic charge transport through the molecule, and on the analysis of the phenomenon of vibrational instability. This analysis leads to new strategies for overcoming the excessive vibrational heating during resonant transport, including counter-intuitive effects, such as high-voltage assisted mechanical stabilization [1], and high temperature stabilization ("cooling by heating" [2]). These results are explained using an analytical model and are demonstrated to hold beyond the model limitations using numerical simulations. This work provides some guidelines for cooling nano-scale conductors operating in the resonant tunneling regime, as well as some practical suggestions with respect to experimentally controlled parameters that can be tuned in order to enhance the mechanical stability of nano-electronic devices.

[1] D. Gelbwaser-Klimovsky, A. Aspuru-Guzik, M. Thoss, and U. Peskin, High voltage assisted mechanical stabilization of single-molecule junctions, Nano Lett. 18, 8, 4727 (2018).

[2] R. Härtle, C. Schinabeck, M. Kulkarni, D. Gelbwaser-Klimovsky, M. Thoss and U. Peskin, Cooling by heating in nonequilibrium nanosystems, PRB 98, 081404(R) (2018).