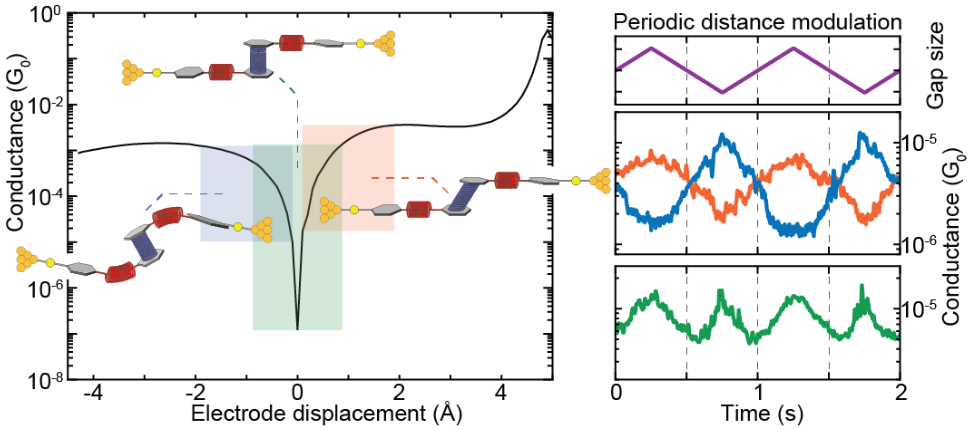
Large Conductance Variations in a Mechanosensitive Single-Molecule Junction

Davide Stefani, Kevin J. Weiland, Maxim Skripnik, Chunwei Hsu, Mickael L. Perrin, Marcel Mayor, Fabian Pauly, Herre S. J. van der Zant

Department of Chemistry, University of Basel, 4056 Basel, Switzerland
kevin.weiland@unibas.ch

The appealing feature of molecular electronics is the possibility of inducing changes in the orbital structure through external stimuli. This can provide functionality on the single molecule level, which can be employed for sensing or switching purposes, if the associated conductance changes are sizable upon application of the stimuli. Here, we show that the room-temperature conductance of a spring-like molecule can be mechanically controlled up to an order of magnitude by compressing or elongating it. Quantum chemistry calculations indicate that the large conductance variations are the result of destructive interference effects between the frontier orbitals that can be lifted by applying either compressive or tensile strain to the molecule.



When periodically modulating the electrode separation, a conductance modulation at double the driving frequency is observed, providing a direct proof for the presence of quantum interference. Furthermore, oscillations in the conductance occur when the stress built up in the molecule is high enough to allow the anchoring groups to move along the surface in a stick-slip-like fashion. The mechanical control of quantum interference effects results in the largest gauge factor reported for single-molecule devices up to now, which may open the door for applications in, *e.g.*, a nano-scale mechanosensitive sensing device functional at room temperature.

[1] D. Stefani, K. J. Weiland, M. Skripnik, C. Hsu, M. L. Perrin, M. Mayor, F. Pauly, H. S: J. van der Zant, *Nano Letters*, **2018**, 10.1021/acs.nanolett.8b02810.