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Tenkých vrstev a nanostruktur

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TÉMA

Azobenzene: From electronic structure to molecular switching*

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Azobenzene (AB) is an iconic photoswitchable molecule and a candidate for light-triggered switches and light-powered molecular machines. Yet, fundamental understanding of electronic structure of AB and AB embedded into functional junctions formed by contacting AB with metal electrodes is still missing.

In order to fill the gap we first study low-energy singlet and triplet states of AB molecule in a hierarchy of accuracies: DFT (Density Functional Theory), gROKS (generalized Restricted Open Shell Kohn Shan), and QMC (Quantum Monte Carlo). While only the QMC method yields quantitatively correct results for the ground- and all excited-states, DFT and gROKS are found to provide qualitatively correct description of the lowest singlet (S_0 , S_1) states. Such a treatment can be made even quantitatively correct by application of a uniform blue shift of +0.7 eV to the lowest gROKS excited states energies.

We further study AB embedded into junctions by the DFT/gROKS techniques. The ability of anchored photoswitches to perform optically, mechanically, and opto-mechanically driven switching cycles is studied. As a model for such nanoscale devices we have simulated molecular switches consisting of a single dithioazobenzene bridge between gold tips, Fig. 1. Purely optical switching cycles are hindered by mechanical effects due to the tips. However, the possibility of performing both combined opto-mechanical and purely mechanical two-way switching is predicted.

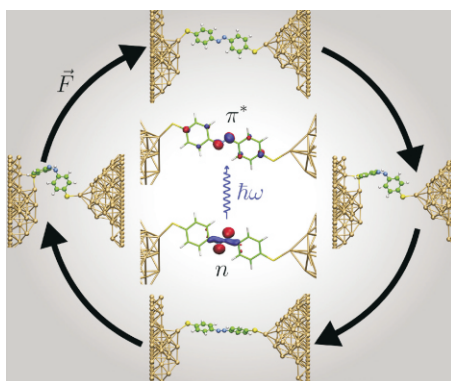


Fig. 1. Schematics of mechanical and optical switching cycles.

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