SYSA 6: Organic Interfaces (further abstracts see DS 19.2-11)

Time: Wednesday 14:30–17:30 Location: H 2013

Invited Talk SYSA 6.1 Wed 14:30 H 2013

Organometallic Nanojunctions Probed by Different Chemistries: Thermo-, Photo, and Mechanochemistry — •I. Stich[1,2], M. Konopka[1], R. Turansky[1], J. Reichert[3], N. L. Doltsinis[4], H. Fuchs[3], and D. Marx[4] — [1]Slovak Tech. Univ. (FEI STU), Slovakia — [2]Inst. of Phys., Slovak Acad. of Sci., Slovakia — [3]Uni. Muenster, Germany — [4]Ruhr-Uni. Bochum, Germany

Different methods of activation of chemical reactions are compared for organometallic nanojuctions. The study is based on density functional theory simulations. First we provide a comparison of thermal activation with mechanical activation, or mechanochemistry. Study of thiolate/copper junctions and interfaces provides evidence for vastly different reaction pathways and products. The differences are understood in terms of mechanical manipulation of coordination numbers and system fluctuations in the process of mechanical activation. Next we compare photo- and mechanochemistry. Azobenzene is an optically switchable molecule. Laser light is normally used to achieve molecular switching between the cis and trans isomers. We study azobenzene optomechanical switch which combines photo excitation with external pulling force to manipulate optical switching properties of the azobenzene molecule anchored to gold tips by thiolate bonds. We focus on the separation between ground (S0) and first excited (S1) singlet states. We observe a pronounced dependence of the S0-S1 separation on the applied strain. Furthermore we find that ground-state mechanochemistry alone can be used to achieve switching. For instance, mechanochemistry with modest applied forces leads to cis -> trans reisomerization.

Joined session with DS: Further abstracts are listed under DS 19.2-11