

“Electron Injection Dynamics in Au(111)-Molecule Interfaces: A theoretical Study”

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We present a study of electron transfer and electron transport processes in molecular systems at metal substrates. In particular, photoinduced electron transfer in molecules at metal surfaces and voltage driven electron transport in single-molecule junctions are investigated, see Figure 1. The methodology is based on a combination of first-principle electronic structure methods to characterize the systems and dynamical basis-set as well as nonequilibrium Green's function methods to study electron transfer dynamics and transport properties, respectively^[1].

The results show the ultrafast character of electron transfer at molecule-metal interfaces and demonstrate the importance of electronic-vibrational coupling in single-molecule junctions. Furthermore, a mechanism for photoinduced switching of molecular junctions based on hydrogen translocation^[2] is discussed.

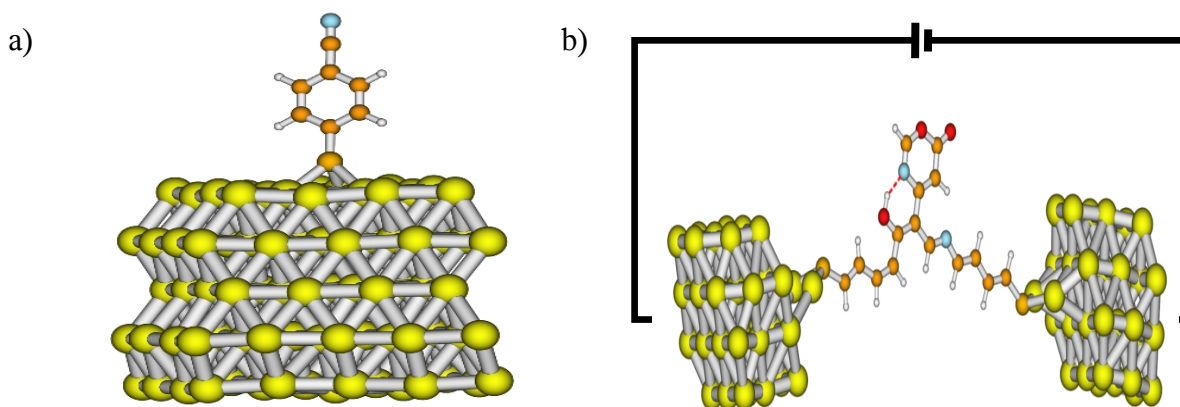


Figure 1. a) Molecule at metal surface and b) single-molecule junction

References:

1. O. Rubio-Pons, R. Härtle, Jingrui Li, M. Thoss, Theoretical Study of Electron Transfer and Electron Transport Processes in Molecular Systems at Metal Substrates. High Performance Computing in Science and Engineering Springer (2010) in press
2. C. Benesch, M.F. Rode, M. Cizek, R. Härtle, O. Rubio-Pons, M. Thoss, and A. Sobolewski Switching the conductance of a single molecule by photoinduced hydrogen transfer J. Phys. Chem. C. 113, 10315 (2009).