Theoretical investigations on the photodesorption of CO on Si(100)

Niklas Thoben, Thorsten Klüner

Carl von Ossietzky University of Oldenburg, Germany

The investigation and understanding of photoinduced processes on solid surfaces on the atomic scale still remains a major challenge even for the simplest of these reactions such as photodesorption. A recent experimental study on the model system CO on Si(100) [1] found a bimodality in the time-of-flight spectra of the desorbing molecules after irradiation with light in the UV/vis-range. The authors assume two photodesorption channels with mean translational energies of 0.260 and 0.111 eV, respectively.

In this contribution, we give a suggestion for the underlying mechanism based on quantum mechanical considerations. After the description of the adsorption of CO on Si(100) in the ground state using hybrid density functional theory and periodic boundary conditions, hydrogen-saturated cluster models were created to calculate several excited states of the CO-Si(100) system using the CASSCF-method. An analysis of the obtained one dimensional potential energy curves of the different states as well as quantum dynamical simulations on those curves allow first conclusions concerning the photodesorption mechanism.

[1] M. Lackner, D. Lucaßen, E. Hasselbrink, *Chem. Phys. Lett.* **2018**, *713*, 277.