Chemistry at the solid-liquid interface

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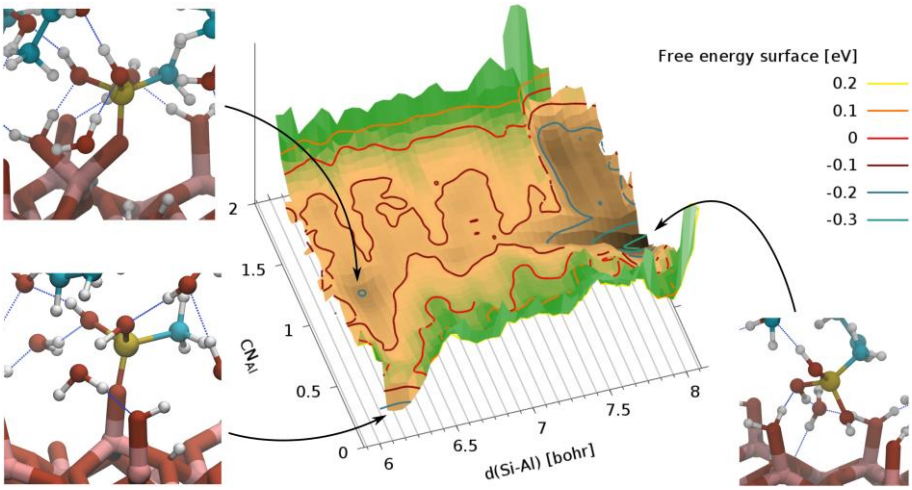

Chemical functionalization of surfaces, i.e. the covalent attachment of molecules, is usually done by wet-chemical processes. In our research we use *ab initio* molecular dynamics (AIMD) together with acceleration techniques such as metadynamics to obtain fundamental insights into the mechanisms of molecular adsorption, reaction and binding at such solid-liquid interfaces. This will be illustrated by two examples, the anchoring of a typical silanol linker unit to aluminum oxide via condensation reactions in the presence of liquid isopropanol and the oxidation chemistry of graphite by intercalation with liquid sulfuric acid.

In the first example we will focus on the identification of relevant transition state structures, the role of residual water at the surface and the impact of proton dynamics at the interface. For the intercalated graphite we will discuss the stability of oxygen species in the presence of sulfuric acid and we show that oxidation and ideal crystallinity reduce the molecular friction and thereby facilitate a fast and efficient intercalation [1]. The graphite intercalation compound furthermore serves as a well-defined model system of a confined liquid for which we studied the impact of confinement on the dynamics of the liquid, the stability of the hydrogen-bond network and the kinetics of proton diffusion. These time consuming AIMD simulations only became possible with our recent improvements in the Car-Parrinello Molecular Dynamics (CPMD) code [2].

[1] S. Seiler, C.E. Halbig, F. Grote, P. Rietsch, F. Börrnert, U. Kaiser, B. Meyer, S. Eigler, Effect of friction on oxidative graphite intercalation and high-quality graphene formation, *Nature Commun.* **2018**, *9*, 836

[2] T. Klöffel, B. Meyer, G. Mathias, Boosting Performance and Scalability of Ab Inito Molecular Dynamics on Multi- and Manycore Architectures, submitted to *Parallel Computing*