

Dynamics of proton transfer reactions on Si(001)

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The reaction of organic molecules on semiconductor surfaces is a fundamental step on the way to hybrid structures with high functionality. For this reason, the adsorption of organic molecules with different functional groups on silicon surfaces has been studied in detail; however, only limited experimental information is available on the respective adsorption dynamics. On the other hand, the reaction dynamics are integral part of the reaction mechanism and an improved understanding is expected to give access to better control of the reaction [1]. In most cases, the adsorption of organic molecules on silicon proceeds via a metastable intermediate state (Fig.1, left); for methanol, such an intermediate state was also proposed but has not been observed experimentally yet.

In this work, we apply molecular beam techniques in order to investigate the adsorption dynamics of methanol on Si(001). The initial sticking probability s_0 was measured both as a function of surface temperature and kinetic energy of the impinging molecules. It was found that s_0 decreases with increasing surface temperature, indicating adsorption via an intermediate state. However, quantitative evaluation of these results indicates that the conversion barrier from the intermediate into the final state is comparably low. This is interpreted in terms of a proton transfer reaction, which is associated with a substantially lower barrier when compared to, e.g., cleavage of the O-C-bond [1].

The dependence of s_0 on the kinetic energy of the incoming molecules is shown in (Fig.1, right), a continuous decrease of s_0 with increasing kinetic energy is observed. When compared to the dynamics of, e.g., ether cleavage on Si(001) [2], these results indicate that the low conversion barrier for the proton transfer reaction has no significant influence on the adsorption dynamics, and the reaction is mainly determined by the intermediate state. This picture is backed by additional experiments on the dynamics of H₂O dissociation on Si(001), which show comparable results.

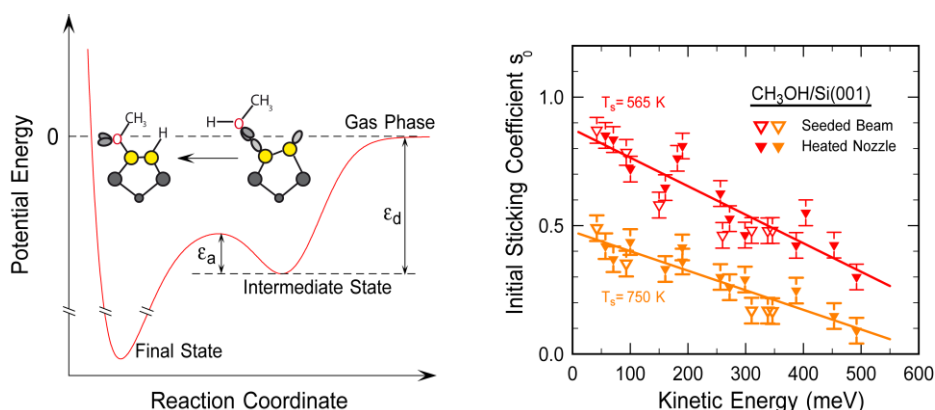


Fig. 1: Left: Schematic potential energy curve for methanol dissociation on Si(001). Right: s_0 as a function of beam energy E_{kin} at two different surface temperatures, s_0 decreases continuously with increasing E_{kin} .

References:

[1] M. Reutzel, et al., J. Phys. Chem. Lett. **6**, 3971 (2015) and J. Phys. Chem. C, **120**, 26284 (2016).

[2] M.A. Lipponer, et al., Surf. Sci. **118**, 651(2016).