O 54: Poster Session - Semiconductor substrates: Adsorption and Reaction of Small Molecules

Time: Tuesday 18:15–20:00 Location: P2/1OG

O 54.1 Tue 18:15 P2/1OG

Vibrational Sum Frequency Generation Spectroscopy Study for Alcohol Adsorption on TiO_2 Thin Film — •Anupam Bera, Denise Bullert, and Eckart Hasselbrink — Fakultät für Chemie, Universität Duisburg-Essen, D-45117 Essen, Germany

The surface chemistry of TiO_2 is most intensely studied as it is seen as a prototype system for its photocatalytic properties in particular in the context of water splitting and pollutant degradation. However, the interaction of TiO_2 with alcohols has attracted less interest although oxidation of the latter is of large industrial relevance. A thorough understanding of the photochemistry requires the fundamental knowledge of composition, structure of the adsorbed alcohols to TiO_2 surface in an ambient alcohol atmosphere at room temperature. However, extracting this important information is the limiting step in the most cases due to the challenges in probing the interfacial molecules at near ambient conditions. To address this limitation, we use vibrational sum frequency generation spectroscopy (vSFS) as it allows to solely detect surface species and discriminates against spurious signals from ambient gas phase. Our present study reveals important adsorption behaviour of the various alcohol (methanol, ethanol and isopropanol) systems on TiO_2 anatase nano thin film under ambient condition. A systematic study utilizing various polarizations and pressure combinations, allowing us to unambiguously assign the adsorbed species. Our findings reveal key insights into the initial mechanistic steps towards heterogeneous alcohol oxidiation reactions at near ambient condition.

O 54.2 Tue 18:15 P2/1OG

Controlled Manipulation of Diethyl Ether on Si(001)via Tip-Induced Electronic Excitation — •Alexa Adamkiewicz[1], Gerson Mette[1], Tamam Bohamud[1], Michael Dürr[1,2], and Ulrich Höfer[1] — [1]Fachbereich Physik, Philipps-Universität Marburg, Germany — [2]Institut für Angewandte Physik, Justus-Liebig-Universität Giessen, Germany

Tip-induced electronic excitation via STM can give access to alternative reaction channels beyond thermal activation. Recently, we showed for the cleavage of tetrahydrofuran (THF) on Si(001) that excitation by the tunneling electrons leads to new final products, which can be selectively addressed by the type of excitation [1].

Here, we present the influence of the detailed configuration of the adsorbates on tip-induced ether cleavage. Due to the linear molecular structure of diethyl ether (Et_2O), the adsorbates undergo fragmentation when cleaved, thus leading to a higher degree of freedom compared to the ring-shaped THF. The final products differ significantly for Et_2O and THF. These differences do not only represent the influence of the different molecular structures of the adsorbates, but also provide insight with respect to the influence of the local electronic structure of the substrate on the reaction and the competition between electronic structure and steric constraints.

[1] G. Mette *et al.* Angew. Chem. Int. Edit. **58**, 3417 (2019).