High Resolution FTIR for Surface Chemistry: Bridging the Pressure Gap

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The recent use of surface sensitive methods has contributed significantly to elucidate the molecular mechanisms of heterogenous catalysis. Necessarily, there are two objections to this approach. First, the surface has to posses a well defined crystalline structure. Second, it is only in the ultra-high vacuum (UHV) domain of reactant gases pressure, that the proposed molecular mechanisms can be ascertained to work.

The materials and pressure ranges involved in real-world catalytic processes do not share any of these features. In popular language, the price paid for using surface sensitive methods is a materials- and pressure gap, respectively. To clarify the relevance of the surface sensitive approach to real catalytic processes, it is necessary to follow these processes by direct observation, on the same substrate in a wide pressure range, extending from UHV conditions up to atmospheric pressure.

In the higher pressure domain optical spectroscopy has to replace the electron spectroscopies (HREELS) customary to the UHV studies. During the last three decades, reflection-absorption infrared spectroscopy (RAIRS) was perfected for the study of layers of molecules adsorbed onto metallic surfaces. The beam is sent at grazing incidence onto the metal substrate, producing an excitation of the molecular electric dipole oscillations normal to the substrate only. The absorption signal carries a wealth of information such as the position of the molecule relative to the substrate and the structure of the adsorbed molecule itself.
For the direct observation of catalytic reactions on surfaces, further specializations of the RAIRS technique are needed. Customarily, RAIRS is used for the study of relatively thick adsorbate films, which could produce alone a sufficient absorption signal. This is not the case with adsorbate layers on catalyzer surfaces, which are at most one molecule thick.

We report here the new RAIRS experimental set up designed for the Bruker IFS 120 HR spectrometer in Giessen.