MODELING THE ACTIVE CENTERS OF CATALYSTS: THE UNIQUE COMBINATION OF GAS-PHASE ION TRAP REACTIVITY AND INFRARED SPECTROSCOPY

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Catalysis represents the key of our modern chemical industry, is essential to reduce waste and air pollution, and plays an important role for solar energy storage as well as electrochemical energy conversion. To direct the optimization of heterogeneous and homogeneous catalysts and to develop new tailor-made catalytic materials a fundamental understanding of the catalytic reactions is indispensable. However, industrial catalysts are typically very complex systems often comprising multiple (nano)materials which render a detailed investigation of the catalytic processes on an atomic and molecular level difficult. To nevertheless gain an essential understanding of catalytic processes, we utilize small (sub)nanometer sized metal, metal-oxide, and metal-sulfur clusters as gas phase model systems. An important aspect that supports the feasibility of such very small isolated systems as catalytic model systems is the fact that catalysis is a local effect and thus generally very restricted to an Ångstrom size atomic area, the so called catalytically active center. These catalytically active centers are typically characterized by unsaturated bonds, like kinks, steps, defects, or very small particles in the sub-nanometer size range and can, thus, be very well modeled by isolated gas phase particles of appropriate size, charge, and material composition. In this talk I will demonstrate the power of gas-phase ion trap reactivity studies in combination with infrared multiple-photon dissociation (IR-MPD) spectroscopy and first-principles calculations to provide a molecular level understanding of fundamental catalytic processes. Particular focus will be on recent spectroscopic studies performed at the free-electron laser facility FELIX (Radboud University Nijmegen, The Netherlands) which are essential for understanding the catalytically active centers of heterogeneous catalysts, biocatalysts, as well as materials of astrochemical relevance.