

Session of Focus Materialchemie – Wednesday, **13.12.2023** 16:00 – @ Seminarraum Lehar 02 (TU-Wien, Getreidemarkt 9, BC, OG. 02, room A46) – [join us](#) on ZOOM (ID: 983 0066 2349)

Ethylene hydrogenation on HOPG supported Ag, Au and Cu: surface science and model catalysis

Thomas Wicht¹, Alexander Genest¹, Thomas Haunold¹, Andreas Steiger-Thirsfeld², Michael Stöger-Pollach², Günther Rupprechter¹

¹Institute of Materials Chemistry, TU Wien, Getreidemarkt 9, 1060 Vienna, Austria

²University Service Centre for Transmission Electron Microscopy, TU Wien, Wiedner Hauptstraße 8-10, 1040 Vienna, Austria

A combined surface science/microreactor approach was applied to examine structure-activity correlations in carbon supported Ag, Au, and Cu nanoparticle catalysts. Spark ablation of the corresponding metals on highly oriented pyrolytic graphite (HOPG) and carbon-coated transmission electron microscopy (TEM) grids yielded nanoparticle catalysts (mean particle size around 3 nm) that are well-suited for characterization by X-ray photoelectron spectroscopy (XPS), high-resolution electron microscopy (HRTEM/STEM) and energy dispersive X-ray spectroscopy (EDX). Polycrystalline metal foils, characterized by scanning electron microscopy (SEM), EDX, electron backscatter diffraction (EBSD), as well as low energy ion scattering (LEIS) served as unsupported reference. Employing a UHV-compatible flow microreactor and gas chromatography (GC) allowed to determine the catalytic performance of the model catalysts in ethylene hydrogenation up to 200°C under atmospheric pressure, yielding temperature-dependent conversion values, turnover frequencies and activation energies. Compared to the pure metal foils, the HOPG-supported metal nanoparticles showed strongly increased activity and stability (slower deactivation), due to better availability of hydrogen at the metal/carbon interface. For the most active Ag catalysts, DFT calculations were additionally carried out to determine adsorption energies of the reacting species on single-crystal surfaces as well as on carbon-supported and unsupported Ag nanoparticles. H₂ adsorption turned out to be substantially facilitated by the presence of a carbon support, mainly due to subtle structural changes of the nanoparticle.