



Sekce chemie PŘF UK v Praze
zve všechny zájemce na přednášku z cyklu

Quo Vadis Chemie

Ménage-à-trois: Single-atom Catalysis, Mass Spectroscopy, and Computational Chemistry



kterou přednese

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v posluchárně CH1, v budově chemických kateder PŘF UK
Hlavova 8, Praha 2

Abstrakt:

We shall present selected examples of gas-phase reactions which are of timely interest for the catalytic activation of small molecules. Due to the very nature of the experiments, detailed insight in the active site of catalysts is provided and – in combination with spectroscopic studies and computational chemistry – mechanistic aspects of as well as the elementary steps involved in the making and breaking of chemical bonds are revealed.^[1]

Examples to be discussed include inter alia: (i) Metal-mediated carbon-carbon bond formation; (ii) low temperature, catalytic oxidation of CO; or (iii) the coupling of NH₃ and CH₄ to produce HCN. Of particular importance are the reactions of "bare" metal-carbene complexes, when generated in the gas phase and exposed to thermal reactions under (near) single-collision conditions.^[2]

[1] For recent references, see: (a) H. Schwarz, *Angew. Chem., Int. Ed.* 2015, 54, 10090; (b) H. Schwarz, *Isr. J. Chem.* 2014, 54, 1413; (c) M. Schlangen, H. Schwarz, *Catal. Lett.* 2012, 142, 1265; (d) N. Dietl, M. Schlangen, H. Schwarz, *Angew. Chem. Int. Ed.* 2012, 51, 5544; (e) H. Schwarz, *Angew. Chem. Int. Ed.* 2011, 50, 10096; (f) D. K. Bohme, H. Schwarz, *Angew. Chem. Int. Ed.* 2005, 44, 2336.

[2] S. Zhou, J. Li, M. Schlangen, H. Schwarz, *Acc. Chem. Res.* 2016, 10.1021/acs.accounts.5b00023.