Christian Papp, Mod Chem Appl 2018, Volume 6
DOI: 10.4172/2329-6798-C2-011

From classical model catalysts to liquid metal alloys

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We present two examples, where fundamental research utilizing XPS provides insight into catalysis and chemical reactions for energy storage. In the first, we investigate the chemical transformation of the norbornadiene/quadricyclane energy storage system on various metal surfaces. The energy in this system is stored by chemical means in the form of strained organic molecules, e.g. the multi-cyclic hydrocarbon quadricyclane (QC) and its strain released counterpart norbornadiene (NBD). By absorption of light, NBD is transformed to the energy-rich QC, followed by a catalytic energy release to reform NBD. We investigated the adsorption of QC and its conversion to NBD; in addition, we also followed the decomposition of both over different catalytically active metal surfaces. In our model approach, we observe the conversion of QC to NBD at 170K on Ni(111) and Au/Ni(111), but not for Pt(111) surface, where the reaction occurs already below 120K. The second example concerns liquid binary alloys of Ga and a transition metal supported on porous silica, so called supported catalytically active liquid metal solutions (SCALMS). These catalyst systems are stable and selective alkane dehydrogenation catalysts, which outperform commercial catalysts. The beneficial effects of adding Ga is assigned to the catalyst being in the liquid phase during reaction. We present XPS of liquid Pd-Ga and Rh-Ga alloys with multiple stoichiometries as model systems for SCALMS. We observe a temperature-dependent change in concentration, due to the formation of solid intermetallics, leading to the depletion of the catalytically active transition metal. In the Pd-Ga alloy, Pd is depleted at the surface. Complementary data on the Rh-Ga system will be presented and compared to the Pd-Ga results. Furthermore, we discuss the behavior during the oxidation of the liquid metallic catalysts.

Biography

Christian Papp received his PhD in 2007 from the University Erlangen (Germany) from 2008-2009, he was a Postdoctoral fellow at the Material Science Division of Lawrence Berkeley National Laboratory. In September 2009 he returned to Erlangen and finished his habilitation there in 2015. At the moment he is group leader of the Surface and *in situ* spectroscopy group at the Chair of Physical Chemistry II at the University of Erlangen Nuremberg. His current research interests are the *in situ* spectroscopic investigation of surface reactions and model catalysis, in particular, hydrogen storage applications and chemically modified graphene.

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