



MAX-PLANCK-GESELLSCHAFT



VIII International Conference „ Mechanism of Catalytic Reactions" 2009

Increased selectivity of Pd based catalysts in alkyne hydrogenation reactions by the modification of their electronic structure

D. TESCHNER, K. KOVNIR, M. HÄVECKER, Z. RÉVAY*,
A. KNOP-GERICKE, M. ARMBRÜSTER[#], Y. Grin[#], R. SCHLÖGL

**Institute of Isotopes, 1525 Budapest Hungary*

[#]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Fritz-Haber-Institut der Max-Planck-Gesellschaft, Dept. Inorganic Chemistry, Faradayweg 4-6, 14195 Berlin, Germany

knop@fhi-berlin.mpg.de

Palladium based catalysts are used for selective hydrogenation of alkynes to alkenes. Modifications of the near-surface region either by the incorporation of carbon on interstitial lattice sites or by the application of Pd intermetallic compounds cause an increased selectivity compared to pure Pd. Under reaction conditions of the total hydrogenation much less carbon is dissolved in the Palladium as shown by in situ photoelectron spectroscopy [1-3]. In situ prompt γ activation analysis studies indicated that unselective hydrogenation proceeds on hydrogen-saturated β -hydride, whereas selective hydrogenation was only possible after decoupling bulk properties from the surface events.

The structurally well-defined intermetallic compound PdGa - highly selectivity for the selective hydrogenation of acetylene- show a strong modification of the electronic states on the surface of PdGa compared to elemental Pd and a complete isolation of the Pd atoms on the surface of PdGa. In situ investigations proved the high stability of the surface, thus excluding segregation phenomena (common for alloys) or sub-surface chemistry involving C and/or H atoms (known for elemental Pd) [4]. By suppressing the sub-surface chemistry, the electronic modification as well as the site isolation leads to high selectivity and long-term stability of PdGa in the selective hydrogenation of acetylene.

References:

- [1] D. Teschner, E. Vass, M. Hävecker et al.; J. Catal. 242, 26, 2006
- [2] D. Teschner, J. Borsodi, A. Wootsch, Z. Révay et al.; Science 320, 86, 2008
- [3] D. Teschner, Z. Révay et al.; Angew. Chem. Int. Ed. 47, 9274, 2008
- [4] K. Kohnir, M. Armbrüster, D. Teschner, T. V. Venkov et al.; Surf. Sci. 2009