



Vortragsankündigung

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Es spricht: **Prof. Dr. Horia Metiu**, Department of Chemistry and Biochemistry, University of California, Santa Barbara

Zeit: **Mittwoch, 15. Juli 2009 17:15 Uhr**

Ort: **TU Berlin**
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Raum C 243

Thema: **Catalyst activation by molecular sized centers**

Abstract: Oxides are widely used as catalysts for partial oxidation, oxidative dehydrogenation and ammoxidation. We use density functional theory to examine to what extent we can increase the activity and the selectivity of these catalysts by creating on their surface molecule-sized centers chosen to disrupt the chemical bonding at the surface. We examine here two such disruptions: (a) substitutional doping of a fraction of the cations on the oxide surface with other cations and (b) the deposition of very small oxide clusters on an oxide support. We show that doping oxides can substantially change their catalytic properties.

We have identified four mechanisms: 1. The dopant activates the surface oxygen atoms nearby and speeds up oxidation by a Mars-Van Krevelen mechanism; 2. The dopant adsorbs an O₂ molecule from the gas-phase and weakens its O-O bond making it a good oxidant. 3. The dopant and a surface oxygen atom nearby are both activated helping the dissociative adsorption of molecules; 4. The dopant takes oxygen atoms from the oxide surface and activates them, making them good oxidants. We have also examined the mechanism by which the clusters of molybdenum oxide, vanadium oxide and chromium oxides break the C-H bond during the oxidation of methanol to formaldehyde.

Organisator: **Prof. Dr. Matthias Scheffler**, Fritz-Haber-Institut (MPG)
Gäste sind herzlich willkommen!

Prof. Dr. Matthias Driß
Sprecher des Exzellenz-Clusters UniCat