Course: From supported clusters to nanocatalysis

Part I Catalysis by supported metal clusters and model systems

This talk enters in the field of catalysis by supported clusters, and introduces the idea of model systems in UHV, i.e. of real systems where the complexity of a heterogeneous catalyst is reduced in order to control the parameters which determine the chemical activity. Topics covered: oxide supports, preparation of nanoparticles, characterization tools, examples of reactivity.
Level: Master and PhD Students

Part II - CO on MgO: lessons from 25 years of interplay between theory and experiment (the role of surface science)

Understanding the properties of supported clusters requires a detailed knowledge of the morphology of the support, usually an oxide surface. This entertaining lecture gives the true story of a quarter of a century of efforts to understand the surface of a simple oxide, MgO. It is also a nice example of how science proceeds in these days. Topics: experiments on MgO powders, MgO thin films, MgO single crystals, early calculations (HF, CI) with cluster models, DFT calculations with supercell approaches. An overview of the advancement of quantum theory in the description of oxide materials in the 80's and 90's.
Level: Master and PhD Students

Part III Oxide surfaces: role of morphology, defects, sample preparation

A classical lecture discussing the most important problems connected with oxide surfaces. The aim is to show the complexity of oxide surfaces, and the experimental tools available to investigate them. This is essential in order to control the activity of a nanocatalyst. Topics: oxide morphology and chemical reactivity, characterization tools (AFM, STM, phonons), defects electronic structure.
Level: Master and PhD Students

Part IV The unusual properties supported gold: size, charging, support effects

This talk describes the surprising discovery of the catalytic activity of nanostructured gold, and introduces the important concepts of interaction with the oxide support and consequent charging of the metal cluster. It also contains a nice story of interplay between theory and experiment. Topics: the Haruta catalyst, role of charging in modifying the properties of a nanoparticle, measures of charging, CO vibrational spectra, role of theory.
Level: Master and PhD Students

Part V New phenomena: metal clusters on ultra-thin oxide films

This research talk deals with supported metal nanoparticles. It contains a review of the results obtained in our lab in the last 4-5 years and of the experiments performed in the group of H.J. Freund at the Frtiz-Haber Instituti in Berlin on ultrathin oxide films and supported gold clusters. It reports nice examples of interplay between theory and experiment. It is closely related to the rest of the talks but it can be given independently. Topics: different and unusual properties of gold atoms and clusters on oxide ultrathin films; charging mechanisms; engineering of metal/oxide interfaces; work function changes at metal/oxide interfaces; STM images and their interpretation.
Level: PhD Students post-docs, faculty members

Part VI Photoactivity of titanium dioxide nanoparticles: from basic aspects to applications

This talk presents a general review of the use of titania in applications related to the harvesting of solar light. After an historical review, the basic principles of electrons-holes generation by light absorption are introduced. Possible applications, from water splitting to self-cleaning surfaces, from antibacterial activity to photocatalysis, are discussed. The problem of shifting the activity of titaniaparticles from UV to visible region by doping with heteroatoms or by adding dye molecules (Graetzel cells) is presented. It is shown that the electronic properties of TiO_2 nanoparticles are largely related to the presence of defects introducing gap states. The description of these defects with first principles methods like presents problems due to the self-interaction error. The existence of localized and delocalized states very close in energy makes the problem even more complicated, even when methods like DFT+U or hybrid functionals are used. Comparison with experiment (EPR, XPS, EELS, etc.) is required to gain understanding on this materials.
Level: Master and PhD Students