IAP Seminar

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Tuesday, 5th February 2019, 10:30 s.t.
TU Wien, Institut für Angewandte Physik, E134
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Yellow Tower „B“, 5th floor, SEM.R. DB gelb 05 B

Cerium Oxide Surfaces: Defect Structure and Their Role as Support in Catalysis – A Theoretical Perspective

Ceria (CeO_2) is the most significant of the oxides of rare-earth metals in industrial catalysis. Deep understanding of the oxygen defect structure of ceria surfaces under reducing conditions is essential to tailor their functionality in catalytic applications. For the CeO_2(111) surface, whether oxygen vacancies prefer the subsurface or the surface and if surface oxygen vacancies attract or repel, are still heavily debated. Also, a number of ordered phases have been observed upon reduction, namely, (√7 × √7) *R*19.1º, (√7 × 3) *R*19.1º, (3 × 3), (√3 × √3) *R*30º, and (4 × 4), but their structures have remained elusive. Here, supported by experimental and theoretical results, the current understanding of the structure of the CeO_{2-x} (111) surface will be discussed [1-6].

Furthermore, the role of ceria as support in the catalytic activity of metal-ceria systems is not fully understood. Its non-innocent role will be here discussed using ceria-supported metal nanoparticles as experimental and theoretical model catalysts. Co- and Ni-ceria systems will be used as examples of catalysts for methane dry reforming with CO_2 to produce syngas, a relevant process from the environmental standpoint [7-9]. Ni-ceria will also be considered for hydrogen production [10] and the direct conversion of methane to methanol [11].

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All interested colleagues are welcome to this seminar lecture (45 min. presentation followed by discussion).

Friedrich Aumayr (LVA-Leiter)

Ulrike Diebold (Seminar Chair)