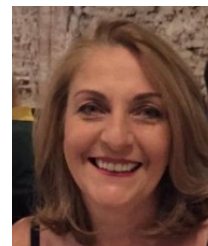


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Tuesday, 5th February 2019, 10:30 s.t.

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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 $\text{CeO}_2(111)$ 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, $(\sqrt{7} \times \sqrt{7}) R19.1^\circ$, $(\sqrt{7} \times 3) R19.1^\circ$, (3×3) , $(\sqrt{3} \times \sqrt{3}) R30^\circ$, and (4×4) , but their structures have remained elusive. Here, supported by experimental and theoretical results, the current understanding of the structure of the $\text{CeO}_{2-x}(111)$ 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)