Contribution ID: **9** Type: **not specified**

Oxygen storage in CeO2/Pt: XAS and DFT studies

Thursday 22 May 2014 09:45 (30 minutes)

In the last decades, media have talked a lot about a very serious thematic as environmental and energetic problem. This thesis is going to show the study on CeO2 as one of the possible candidate for both cases. The importance of ceria is given by its ability to store and release oxygen reversible. Main purpose of this work is to understand low temperature oxygen storage capacity (LT OSC) mechanism and the related structure of the reduced ceria surface on the atomic scale. The sample used is CeO2 nanorods promoted with Pt nanoparticles at different chemical environments and temperatures and, as references, CeO2 from NIST (National Institute of Standards and Technology), CeO2 rods, CeAlO3, Ce2Zr2O7. The CeO2 is considered for Ce4+, CeAlO3 for Ce3+, and instead in Ce2Zr2O7 both Ce3+ and Ce4+ are present. There were performed HERFD XANES spectra at the Ce L1 and L3 edges measured at the SuperXAS beamline at SLS (PSI, Villigen, Switzerland) and soft X-ray absorption Max Lab II (Lund, Sweden) at I1011 beamline at Ce M4 and M5 edges and at O K edge. In order to study the LT OSC process theoretically the DFT simulations were carried out using pseudopotential plane wave approximation within VASP software. Following structures were considered used in simulations: pure CeO2 bulk, CeO2 (111) surface, Ce2O3 hexagonal and cubic, Ce11O20, Ce7O12 and 2x2x2 supercell of CeO2 with O vacancy. Atomic structure, DOS and bandstructure has been derived and then compared with experimental data.

Author: BRAGLIA, Luca (Torino University, Southern Federal University)

Co-authors: Dr GUDA, Alexander (Southern Federal University); Prof. SOLDATOV, Alexander (Southern Federal University)

Presenter: BRAGLIA, Luca (Torino University, Southern Federal University)

Session Classification: Student Sessions