High Resolution Electron Energy Loss Spectroscopy of CeO2

<u>Agata Plucienik^a</u>, Kristin Werner^b, Helmut Kuhlenbeck^c and Hajo Freund^d Authors ^{a,b,c,d}- Fritz-Haber-Institut der Max-Planck-Gesellschaft Author Email: plucienik@fhi-berlin.mpg.de

Cerium dioxide (CeO2, ceria), has attracted much attention in heterogeneous catalysis, which is due to the fact that without major structural transformations, it is possible to simply reduce Ce4+ ions to Ce3+ in a reversible way. According to that process, CeO2 can serve as an oxygen storage-and-release reservoir, which makes it a perfect supporting material in a variety of oxidation reactions. The mechanism of the selective hydrogenation reaction over CeO2 has been studied theoretically and investigated experimentally, however further evidence is required. The results of previous IR spectroscopy and NRA studies revealed that on the stoichiometric CeO2 (111) surface, H species are mostly located on the oxide surface as hydroxyls. In the case of reduced CeO2-x (111) thin films, H species can be found in the bulk volume, as well as the surface. High-resolution electron energy loss spectroscopy (HREELS) is a popular technique, which is mainly used to obtain the vibrational signature of surface and adsorbate species under ultrahigh vacuum conditions. By assigning the vibrational modes, it is possible to confirm previous results on CeO2 (111). Moreover, we noticed that depending on the reduction state of the film, and dosing parameters, ceria can store large amounts of hydrogen, which stabilizes the structure. By using TPD and DFT methods, we are able to identify hydrogen species. Future experiments will focus on both the morphology of the film and possible reactions using the hydroaen reservoir.

References

[1] García-Melchor, M.; Lopez, N. J. Phys. Chem. C 2014, 118, 10921.

[2] Vile, G.; Bridier, B.; Wichert, J.; Per ez-Ramírez, J. Angew. Chem., 644 Int. Ed. 2012, 51, 8620.

[3] Werner, K.; Weng, X.; Calaza, F.; Sterrer, M.; Paier, J.; Sauer, J.; Wilde, M.; Freund, H-J.; J. Am. Chem. Soc., 2017, 139 (48), pp 17608–17616.