”Ab initio” study of interface Cu-Ce-O

Abstract: The present work is a theoretical analysis based on the numerical DFT+U simulations investigating the structural and electronic properties of Cu/CeO_2 model systems, which have important applications as heterogeneous catalysts for environment protection and energy sources. We provide a detailed insight into the cohesion of the interface between metal Cu nanoparticles supported on CeO_2 substrates. This issue is analyzed both in context of small supported Cu clusters as well as for the extended interface underneath Cu nanoparticles on ceria surfaces.
These cases were modelled with a $Cu(111)/CeO_2(111)$ interface and with a Cu adatom adsorbed at the oxidized and reduced $CeO_2(111)$ surface, respectively. The thesis provides a direct correlation between the cohesive and electronic properties mediated by the charge transfer process.
The reduction of surface cerium atoms in the presence of copper either in form of adatom, thin copper layer or a slab of copper is predicted to result from charge transferred from the metal. Since cerium reduction is suggested to play an important role into the catalytic activity of ceria-based catalysts, by predicting the reduction of cerium ions in the presence of copper it can be expected that Cu/CeO_2 systems will have important applications in catalytic technology.