

The present work is focused on a theoretical analysis based on the numerical DFT+U calculations investigating structural and electronic properties of mixed oxide Sn/CeO₂. The main reasons for this study are reported improved catalytic properties of this system that are most probably caused by catalytic properties of cerium oxides, which are based on releasing or (re)capturing of oxygen atoms via the process of cerium oxidation and reduction. In this work we study compounds of cerium and tin that compose Sn/CeO₂ – that is a metal Sn and CeO₂ together with other compounds SnO₂ and Ce₂O₃ – especially by means of band structures and densities of states. Furthermore we studied mixed oxide Sn/CeO₂ in terms of electronic structure and morphology. In this work we consider two different modifications of the analyzed system – the first one contains oxygen vacancy whereas the second one stay unchanged. Our study is focused on analysis of influence of tin defect upon properties of CeO₂, mainly its effect on reduction of cerium atoms.