

Title: Chemical reactivity of metal-supported ceria thin films: a density functional study

Author: Lucie Szabová

Department: Department of Surface and Plasma Science

Supervisor: Prof. RNDr. Vladimír Matolín, DrSc., Department of Surface and Plasma Science, FMF, CU

Abstract: The present work is a theoretical analysis based on numerical DFT+U simulations investigating the physical and chemical properties of ultrathin ceria films supported by Cu(111). Such materials exhibit high activity towards several important reactions in heterogeneous catalysis such as water-gas shift and CO oxidation, with important applications also for renewable energy technologies such as fuel cells. We provide evidence of the influence of film thickness on the electronic and structural properties as well as on the reactivity of ultrathin ceria films supported by copper. The calculations combined with scanning tunneling microscopy experiments show that one monolayer thin film of ceria on Cu(111) is charged, strained and contains oxygen vacancies due to the limited thickness of the film. The influence of the film thickness on the reactivity of thin ceria films was explored for the case of water adsorption and dissociation. Significant differences were shown for water adsorption and dissociation on one-monolayer ceria compared to thicker films, in particular the two monolayer film exhibited highest adsorption energies.