Quantum chemical study of adsorption at metal oxide surfaces

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This thesis presents a Quantum Chemical Study of Adsorption atMetal Oxide Surfaces. Ab initio molecular electronic structurecalculations have been carried out using the GAUSSIAN 98 code toexamine: (i) Transition metal atoms on oxide supports density functionalcalculations (ii) CO adsorption on Ni, Pd, Cu and Ag on MgO, CaO, SrOand BaO: Density functional Calculations.The thesis consists of Three chapters scheduled as follow:CHAPTER 1This chapter presents a literature survey and a review of theory:Density Functional Theory (DFT) as well as the methods and simulationtechniques employed in the calculations.CHAPTER 2In this chapter, The adsorption of the transition metal atoms Cu,Ni, Ag, and Pd on F and F+ defect sites as well as on regular O2- positionsof the MgO, CaO, SrO, and BaO (001) surfaces with the help of DFTcalculations employing cluster models has studied. The model clusterswere embedded in simulated Coulomb fields that closely approximate theMadelung fields of the host surfaces, and the adsorption properties havebeen analyzed with reference to the basicity and energy gap of the oxidesupport in addition to orbital interactions. The following conclusions havebeen extracted:• We found that adsorption properties of the F site, which contains apair of electrons, is reminiscent of the properties of the regular O2