

# Transition-metal atom adsorption on an F<sub>s</sub> defect site of MgO (100) and the interaction with a hydrogen atom

Florez, Elizabeth

Mondragón, Fanor

Truong, Thanh N.

Fuentealba, Patricio

The interaction of transition metals belonging to the group Pt-Pd-Ni and the period Ni-Cu-Zn, with an F<sub>s</sub> center of the MgO (100) surface was investigated using density functional theory. This study was aimed at finding the effect of the electron delocalization of an MgO oxygen vacancy on the interaction energies of the metals with the defect and the electronic configuration of the adsorbed metal atom. The degree of electron delocalization was determined from the maximum values of the electron localization function (ELF). It is confirmed that there are two electrons largely localized in the center of the F<sub>s</sub> vacancy. These electrons can delocalize over an adsorbed metal atom. This is the reason for the stabilization of some surface complexes. The MO analysis shows that the filling and the symmetry of the last occupied orbitals of the complex M- F<sub>s</sub>/MgO depends on the kind of metal. In the case of Ni and Pt the orbitals from HOMO until HOMO-4 are d orbitals and the interaction orbital is t