Effect of surface site on the spin state of first-row transition metals adsorbed on MgO: Embedded cluster model and hybrid density functional theory calculations

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The interaction of first-row transition-metal atoms with low-coordinated oxygen atoms and oxygen vacancies of the MgO surface at low coverage has been studied systematically using an embedded-cluster model approach and hybrid density functional theory calculations. It was found that the interaction with these defects is much stronger than with the regular sites but in general insufficient to change the number of unpaired electrons in the free metal atom. Nevertheless, the larger interaction at these sites reduces the energy required to switch from high spin to low spin. These findings are in agreement with previous work on the adsorption of transition-metal atoms on regular anionic sites of the MgO(001) surface. Our results show that the spin state of adsorbed metal atoms on oxide supports needs to be explicitly taken into account.