

FERROMAGNETIC STATES AT THE O SURFACES OF ZnO AND Co-ZnO

N. Sanchez^a, S. Gallego^a and M.C. Muñoz^a

^aInstituto de Ciencia de Materiales de Madrid, CSIC

The nature of the observed high-temperature ferromagnetism (FM) in dilute magnetic oxides remains controversial since FM is strongly dependent on the preparation conditions. Ferromagnetic order is mainly observed in low-dimensional structures, with multiple surfaces and interfaces. Even more important, ZnO doped by non-magnetic elements and undoped films and nanoparticles are ferromagnetic.

We present a first-principles study of the local magnetic order at the (0001) and (000-1) Oxygen surfaces of wurzite Co-doped ZnO, which shows that the presence of the surface enhances the spin polarization induced by Co atoms. Substitutional Co ions develop large magnetic moments, $\sim 3\mu_B$, and induce local spin polarization at the neighbouring Oxygens. The induced magnetic moments are three times larger at the surface than at the bulk, and even for an antiferromagnetic alignment of Co atoms there is an uncompensated ferromagnetic contribution from the surface. Moreover, even in the absence of magnetic ions, a robust ferromagnetic state is predicted for the O-terminated (0001) surface, due to the occurrence of *p*-holes in the valence band of the oxide. *p*-holes mainly reside in the minority spin orbitals perpendicular to the surface and therefore, the magnetic charge distribution is highly anisotropic. Thus, besides the indirect magnetic interaction between Co atoms, low-dimensional structures of Co-doped ZnO may present additional spin polarization associated to uncompensated local Oxygen charge. This result is a general phenomena occurring in simple oxides when local charge compensation is violated.

9.7 cm

13.4 cm

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Corresponding author :

M.C. Muñoz

Address for correspondence :

Inst. de Ciencia de Materiales de Madrid (CSIC)
c/ Sor Juana Inés de la Cruz 3
28049 Cantoblanco, Madrid (Spain)

Email address :

mcarmen@icmm.csic.es