Selected Topics

1. Spintronics
2. Electronic transport

First Principles Electronic Structure Study of Disordered Al, Ti, Mn Doped ZnO

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Recently, extensive research work has been conducted to describe electrical conductivity mechanisms in diluted magnetic semiconductors in order to achieve the control of charge and spin transport in practical devices. In this contribution we present results of a first principles investigation on the electronic structure in wurtzite-type ZnO modified by M= Al, Ti and Mn doping, aimed at disentangling the impurity effects on conductivity and magnetism in these disordered matrices. We carried out self consistent calculations on $M_xZn_{1-x}O$ systems (x=0.02, 0.05 and 0.10) in the Local (Spin) Density Approximation using the FPLO5 band structure code and the BEB-CPA module which treats the chemical disorder in the multiscattering formalism of Blackman–Esterling–Berk [1,2]. We used the exchange and correlations functional in the parameterization of Perdew and Wang [3] and a 16<16<16 integration grid in the Brillouin zone to account for possible Fermi surface effects having in view the donor character of Al and Ti. We performed the calculations at the experimental volume, assumed the impurity substitutional character and considered no lattice relaxation, hence we refer only to the electronic effects due to the substitutions. The calculated densities of states (DOS) show that Al- and Ti-doped materials are already metallic for x=0.02. The Mn-doped system retains its semiconductor character for x up to 0.10; at that concentration it is at the limit of undergoing an insulator-to-metal transition. Our results predict a non magnetic ground state for Al:ZnO and magnetic ground states for Ti/Mn doping. In the Al:ZnO system, the Al 3s and 4s states are partially occupied and form a narrow band localized at the valence band minimum; Al 3s states also contribute to DOS at the Fermi level and hence to conductivity. The exchange-split Ti 3d states are localized at the Fermi level and contribute to both conductivity and magnetism. The Mn majority spin t2g and eg states (fully occupied) are situated in the band gap, whereas the (unoccupied) minority spin states are in the conduction band. In the case of Ti doping the LSDA magnetic moment increases from 0.90 to 1.13 to 1.28 μB/Ti at. for x=0.02, 0.05 and 0.10 respectively (pointing to Ti^{2+} configuration), whereas in the case of Mn the magnetic moment is constant, 4.71 μB/Mn at. (high spin Mn^{2+} configuration) in the whole concentration range. We evaluate the residual resistivity from the present calculated data and discuss our results with reference to various KKR-CPA calculations and experimental data reported on similar systems. References [1] K. Koepernik and H. Eschrig, Phys. Rev. B 59 (1999) 1743. [2] K. Koepernik, B. Velický, R. Hayn and H. Eschrig, Phys. Rev. B 55 (1997) 5717. [3] J. P. Perdew, Y. Wang, Phys. Rev. B 45 (1992) 13244.