Magnetic order of transition-metal δ-doped cubic ZnO

Iosif Galanakis
Department of Materials Science, School of Natural Sciences, University of Patras

The implication of the spin-degree freedom in conventional semiconducting electronic devices offers a new degree of freedom leading to the rapid expansion of the field of spintronics.[1] A plausible route to achieve the implementation of the electrons spin in devices is the doping of semiconductors using transition metal atoms.[2] The interplay between these impurity atoms and the holes/electrons doping of semiconductors can lead to novel magnetic phenomena.

ZnO is a well-known wide-band semiconductor crystallizing in the wurtzite structure which has been widely studied.[3] When grown as a thin film the lattice structure adopted is the cubic zinc-blende structure, while a pressure of about 6 GPa induces the cubic rock-salt structure.[3] ZnO has started to attract considerable attention in spintronic/magnetoelectronic research since it was discovered that the occurrence of Zn/O antisites or defects can lead to the appearance of magnetism.[4]

The properties of transition-metal (V, Cr, Mn, Fe, Co, Ni) δ-doped ZnO are reported based on ab-initio electronic structure calculations where the on-site electronic correlations are included using the Hubbard parameters. Calculated electronic and magnetic properties are considerably altered with respect to usual first-principles band-structure calculations. Most of the studied systems are found to be either half-metals or ferromagnetic/antiferromagnetic semiconductors and thus can be employed in a variety of spintronic applications as spin-filter materials.[5]

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*email: galanakis@upatras.gr

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