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Electronic structure and magnetism of 3d transition metal-doped ZnO nanoribbons: an ab initio study

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Many experimental and theoretical investigations have been reported regarding the 3d transitional metals (TM) doped ZnO dilute magnetic semiconductors (DMS) materials, which have many unique magneto-optical, magneto-electrical, and magnetotransport properties. The integration of DMS materials into today's electronics requires low dimension circumstance in order to make use of the advantages offered by spin. Among nanostructures, nanoribbon (NR) is one kind of one-dimensional nanostructure, thickness of which is much smaller than width. Thus, the confinement effect in a NR is far from uniform in the crosssection compared to its nanowire counterparts. Doping is an efficient approach to tune electrical and magnetic properties of semiconductors.

In this work, we present a theoretical study based on the density functional theory of the electronic and magnetic properties of pure and 3d TMs (Mn, Fe, and Co)-doped ZnONRs with armchair- and zigzag-shaped edges.

Bare and hydrogen-passivated armchair ZnONRs are found to be nonmagnetic semiconductors regardless of their widths. The band gap of aZnONRs decreases monotonically when width increases. Bare zigzag ZnONRs are magnetic with increasing net magnetic moment as width increases. The imbalance between the up and down spin disappears when edges are terminated with hydrogen, which makes hydrogenated zigzag ZnONRs non-magnetic. The band gap and carrier concentration of ZnONRs can be tuned by 3d-TM doping. The formation energies and magnetic moments of ZnO NRs depend from 3d TMs (Mn, Fe, Co) position.

We also investigated the magnetic coupling between the TM ions, and analyze the mechanism of ferromagnetic (FM) coupling and antiferromagnetic (AFM) coupling of TM atoms in the ZnONRs. Also we show that the zinc vacancies affect the FM coupling between the TM atoms.

Our results provide an insight at the atomic level of the electronic and magnetic properties of 3d TM-doped ZnO nanoribbons and pave the way for future applications of ZnO in nanoelectronic and spintronic devices.