Nanocomposites and nanomaterials

First Principles Calculation of Electronic and Magnetic Properties of Bare and Doped ZnO Nanoribbons

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Zinc oxide is the object of an increasing interest in the last years owing to its potential applications in ultraviolet optoelectronics devices, transparent conducting oxide (TCO) thin films and spintronics. For the design and realization of ZnO based devices, one the most relevant issues is doping. This issue is especially important for the application of ZnO as TCO, which necessarily involves the heavy doping with trivalent elements the group III. 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 doped (Ga, In, and Al) 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.

After doped ZnO nanorifbbons, our results clearly demonstrate that the band gap of armchair ZnO nanoribbon increases along with Al, Ga, and In ions occupying Zn sites. The configuration of Al atom replacing Zn atoms is more stable than other doped. The system shows half-metallic characteristics for In-doped ZnO nanoribbons.

These studies provide us with a deep understanding of the novel properties of intrinsic defect ZnO nanoribbons, which is essential to employ ZnONRs as building blocks for the future nanodevices.