ELECTRONIC PROPERTIES OF III-GROUP ELEMENTS DOPED ARMCHAIR ZNO NANORIBBONS

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MOTIVATION

- 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 construction and implementation of ZnO based devices, doping is one of the most applicable issues.
- A great number of different shapes of ZnO nanostructures has been reported: nanorods, nanoribbons, nanobelts, nanowires and nanotubes can be given as examples for 1D structures. Among nanostructures, nanoribbon 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 cross-section compared to its nanowire counterparts
- In this study, we represent based on the density functional theory the theoretical study of the structural, electronic, and optical properties of pure and doped, in particular Ga, In, and Al, ZnO nanoribbons (ZnONRs) with armchair-shaped edge. These studies provide us a deep understanding of the novel properties of doped ZnO nanorribons, which is essential to employ them as building blocks for future application.

MODELS AND METHODS

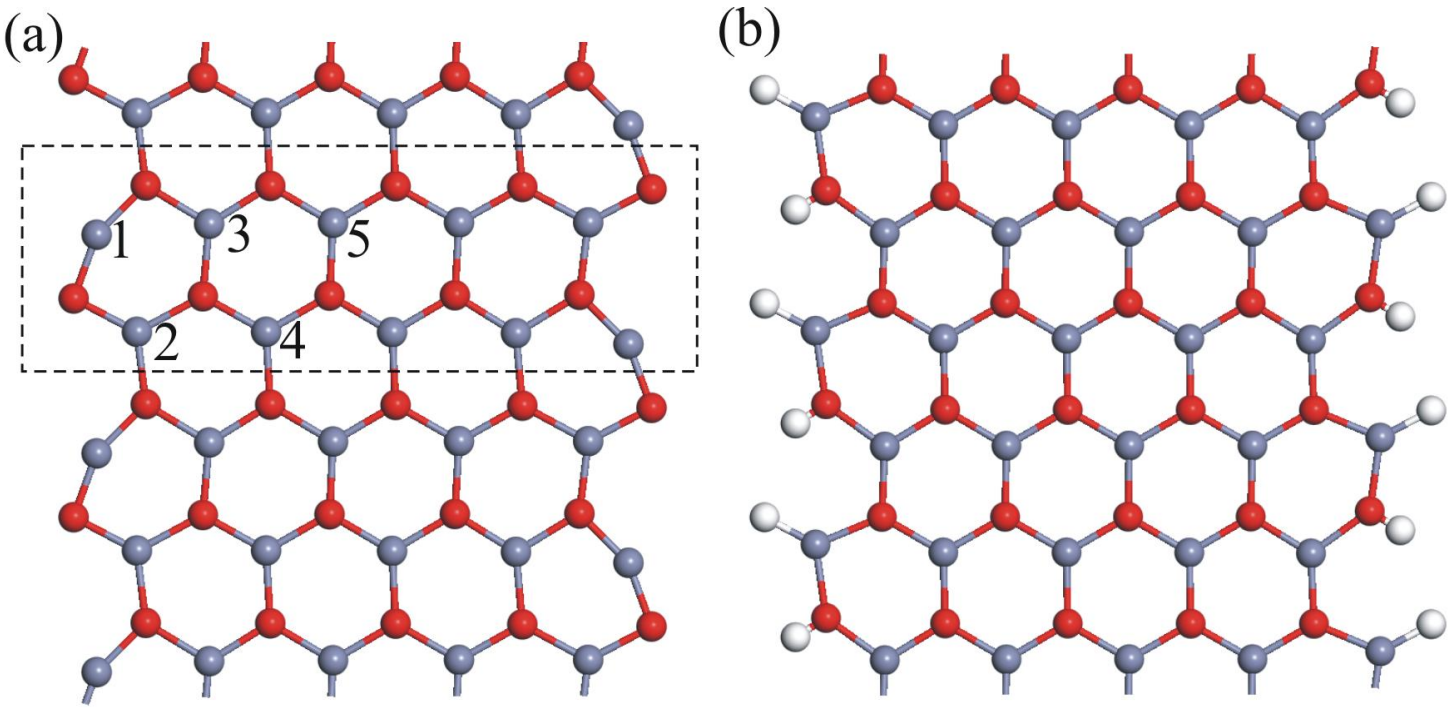
Geometry optimization and electronic structure calculations are performed using the density functional theory (DFT) code. The Perdew-Burke-Ernzerhof (PBE) form of the generalized gradient approximation (GGA) is adopted to describe the exchange correlation interaction. To describe the electronic structures more accurately, we used GGA+*U* method. In this study, we used two values *U*: U_d for 3d orbitals Zn and U_p for 2p orbitals O.

Nanoribbon surfaces were represented in periodic supercells with at least 10 Å of vacuum gap between non-interacting neighboring cells. We consider bare, as well as hydrogen and fluorine saturated armchair nanoribbons. These nanoribbons are specified by their width *w* in Å or *n* number of Zn-O basis formula units in the unit cell. We take armchair nanoribbon with *n* = 10 as prototype.

To simulate various concentrations of dopant (Ga Al, In), this study considered 1×1×2, and 1×1×1 supercells, in which one Zn atom is substituted with one dopant atom, corresponding to doping levels of 5, and 10 %, respectively.

MODELS OF ARMCHAIR ZNO NANORIBBONS

Supercell 1×1×1



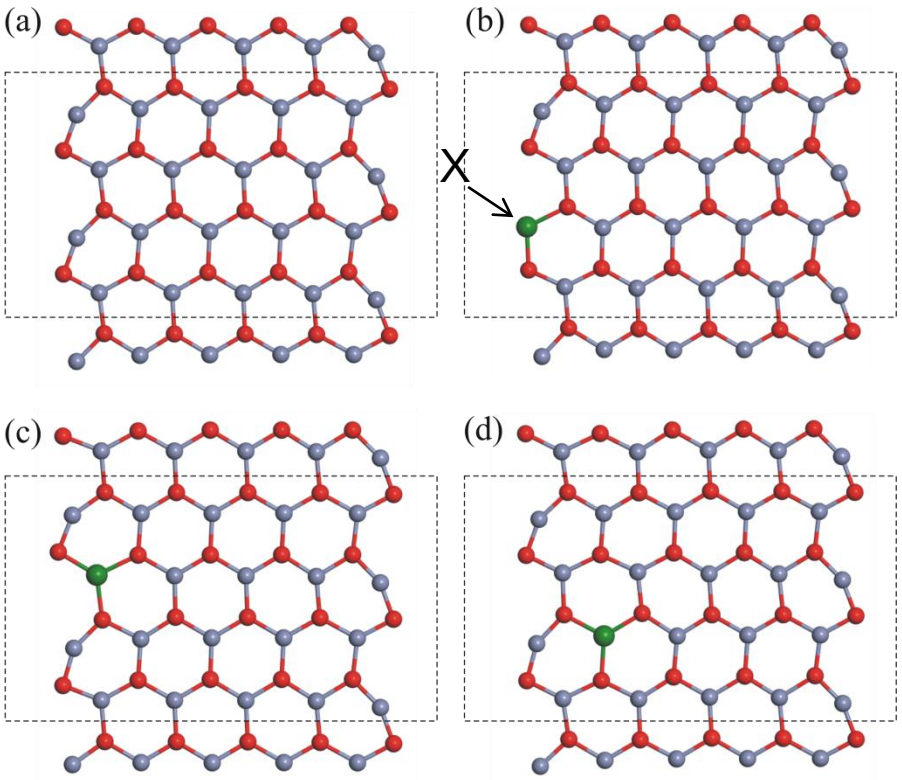
Pure 10-aZnONR

H-passivated 10-aZnONR

Five substitution sites are considered (Fig. (a)) for 10-aZnONRs with dopant atoms.

MODELS OF DOPED ARMCHAIR ZNO NANORIBBONS

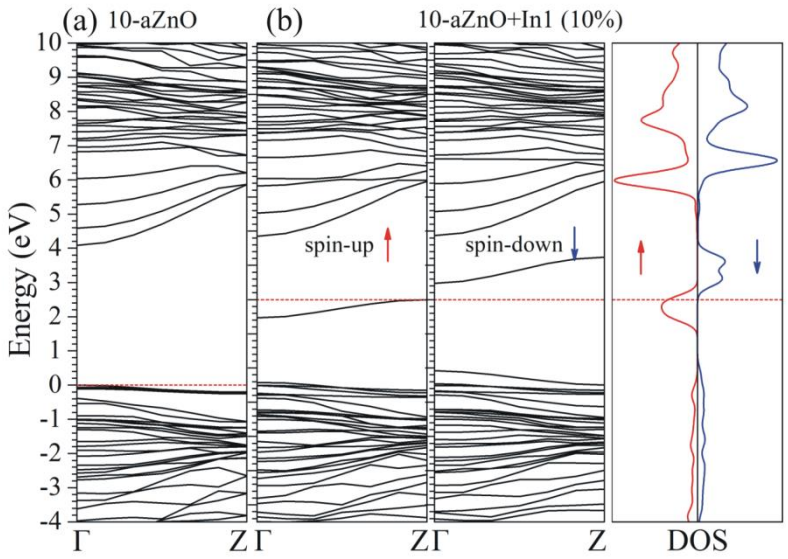
Supercell 1×1×2



X= Al, Ga, In

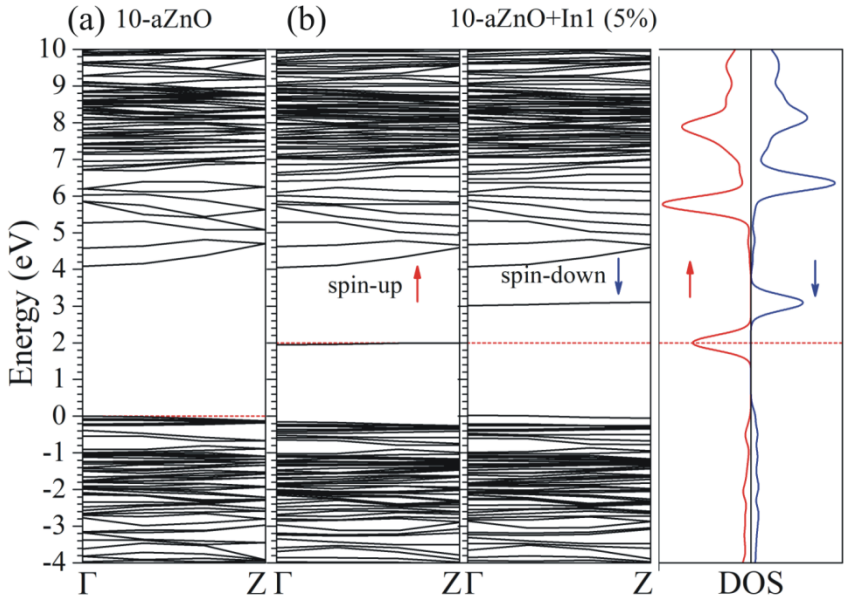
We calculated the formation energy for all substitution position of the dopant atoms, and founded that formation energy is largest when dopant atom occupies position 1. Thus, the configuration 1 is the most favored (Fig. (b)).

ELECTRONIC PROPERTIES OF DOPED 10-AZNONR: IN



In Figure we show the calculated band structure and partial density of states (PDOS) for both pure and In doped (10 %) in different positions of substitution 10-a ZnONRs used GGA+*U* method. In all cases, spin polarization is evident in the band structure and PDOS. Fig. a shows that 10-a ZnONR is a direct band gap semiconductor with a band gap of 4.088 eV at the Γ point. Following the replacement of the Zn atom with the In atom (Fig. (b)), the electrons occupying the lowest level of the conduction band cause the Fermi level (E_F) to move upward into the conduction band, which produces typical n-type characteristics. It is important to note that the E_F is largely crossed by spin-down states, while spin-up states only cut E_F from the right figure, which indicates that the system belongs to half-metallic ferromagnet. In the spin-down states, the impurity bands introduced by In-doped occupy the energy level at the bottom of the conduction band minimum, which shows that In-doped 10-aZnONRs can lead ZnO to an n-type semiconductor.

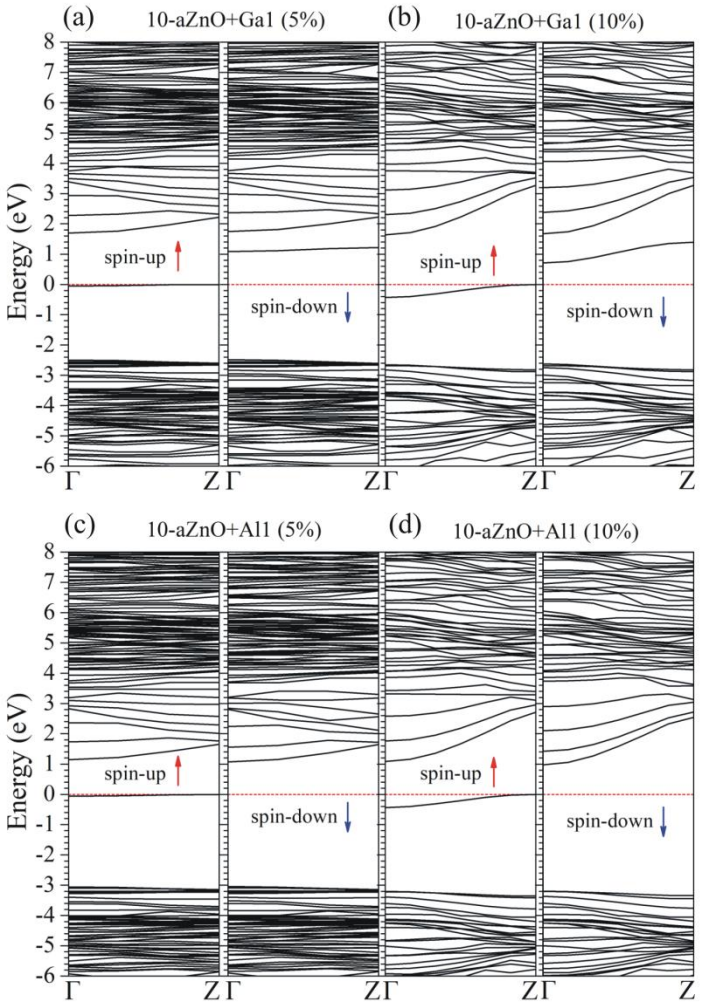
ELECTRONIC PROPERTIES OF DOPED 10-AZNONR: IN



From Figure we can see that the lower the doping concentration of In (5 %), the narrower E_{gO} in 10-aZnONR is (2.16 eV). But behavior spin-up and spin-down states is similar to the higher doping concentration of In.

ELECTRONIC PROPERTIES OF DOPED 10-AZNONR: GA,AL

The Al and Ga doped 10-aZnONRs has optical band gap of 3.09 eV and 2.50 eV for 5 at % concentration. Comparing the band structure of the pristine 10-aZnONR, we observed that the band gap of Al and Ga doping 10-aZnONR decreases. However, for 10 % Al and Ga concentration the E_{gO} increases to 3.20, and 2.65 eV, respectively. The Fermi level shifts toward the conduction band. As the states below such shifting in the conduction band are filled, the absorption edge shifts to higher energy, resulting in a larger band gap. These received values for optical band gaps are higher than that of the In doping nanoribbons



CONCLUSIONS

We have investigated structural and electronic properties of bare and Al, Ga, In-doped armchair single-layer ZnO nanoribbons by first-principles density-functional theory incorporating the GGA and GGA+*U* formalism. All bare and edge-terminated armchair ZnONRs is found to be nonmagnetic semiconductors regardless of their widths.

We find that electronic spectra aZnONRs doped by In, Al, Ga atoms, shows half-metallic character and leads ZnO nanoribbons to an n-type semiconductor. The highest optical band gap is Al-doped aZnONR with concentration 10 %.

The received results are first step for deeply understanding electronic structure ZnO nanoribbons for their potential application in nanoelectronic devices.