Nanocomposites and nanomaterials

Electronic properties of zinc oxide nanoribbons: a DFT study

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ZnO has the richest family of nanostructures among semiconducting oxides and other materials. In terms of production, the synthesis of nanoribbons and nanobelts are easier with respect to nanowires and nanorods having applications in gas sensors. The edges of the ZnO nanoribbons, namely zigzag and armchair, give rise to different electronic, magnetic properties and mechanical properties.

We report a quantum mechanical description based on the density functional theory (DFT) of the structures and electronic properties of zinc oxide nanoribbons (ZnONRs). We consider bare, hydrogen (H) and fluorine (F) passivated armchair and zigzag ZnONRs.

Geometry optimization and electronic structure calculations are performed using the DFT code in which each electronic wave function is expanded in a localized atom-centered basis set defined on a numerical grid. We performed all-electron calculations with a double numeric polarized (DNP) basis set and the gradient-corrected PBE functional. Nanoribbon surfaces were represented in periodic supercells with at least 10 Å of vacuum gap between noninteracting neighboring cells, and accurate Brillouin zone integration was performed via careful sampling of k points chosen according to the Monkhorst-Pack scheme with a k-point spacing of 0.1 $Å^{-1}$.

The following results and conclusions are obtained:

- the bare, H- and F-terminated armchair ZnONRs are nonmagnetic semiconductors with direct band gaps which are relatively larger than that of the monolayer ZnO;
- the band gaps of ZnONRs vary with their widths. The narrow NRs have relatively larger band gap due to the quantum confinement effect;
- the zigzag ZnONRs with or without passivation exhibit small magnetic responses independently of the width. The half-metallicity can be achieved in the ZnONR when and only when edge Zn atoms are passivated by H or F atoms.

These results can be extrapolated to wide ribbons providing a qualitative way of determining the electronic properties of ribbons with widths of practical significance.