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# Electrical properties of two-dimensional zinc oxide in hexagonal, (4,4)-tetragonal, and (4,8)-tetragonal structures by using Hybrid Functional calculation

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Two-dimensional (2D) material is a specific type of materials with its thickness being thinned down to single atomic layer. In many materials, their 2D sheets have been reported to yield very different physical properties from those of their ordinary bulk and other forms of nanostructures. For instance, the band gap of 2D semiconductor sheets can vary from zero band gap (semi-metals, e.g., graphene) to wide band gap insulator (e.g., BN sheet). Among many available metal oxide semiconductor, the monolayer zinc oxide possesses many intriguing properties, such as wide band gap, high charge carrier mobility, being flexible and inherited optical transparency, so it has become a new generation semiconductor of flexible and transparent optoelectronics. However, the growth of the 2D structure in typical semiconductors is very difficult to control as appropriate synthesized technique for such the structure is not well established yet. Specifically, the synthesis route to form the ultrathin 2D material requires breaking of crystal symmetry and fostering of anisotropies in crystal growth. However, successful epitaxial growth of ZnO monolayer in hexagonal structure on graphene substrate was recently achieved and reported to have band gap up to 4 eV. In addition, sub 100-nm-sized ZnO nanosheet in hexagonal wurtzite and tetragonal structures were also found to successfully grow in the solution synthesis using surfactant molecules as a facet at the water-air interface. These then illuminate some possibilities in nano-engineering the structure to achieve ultrathin semiconductor with desired properties. However, the guidelines to comprehend this structure-property relationship should be firstly established. Therefore, in this work, the two-dimensional zinc oxides were studied in tetragonal and hexagonal structures. The electronic calculation was performed using Heyd-Scuseria-Ernzerhof (HSE) hybrid density functional, which mixes the exact non-local exchange of Hartree-Fork (HF) theory with the local exchange and correlation potential of Perdrew-Burke-Ernzerhof (PBE) functional from generalized gradient approximation (GGA). The calculation results showed that the band gaps of 2D ZnO structures are 4.20 eV in hexagonal, 3.06 eV in (4,4)-tetragonal, and 4.59 eV in (4,8)-tetragonal structure, respectively. In term of structure stability, the hexagonal ZnO has more energetic favorable than both of (4,4)- and (4,8)-tetragonal ZnO for about 5.10 eV and 3.15 eV. The small energy differences between these 2D ZnO phases suggest that the phase transformation between these structures is reversible, suggesting band gap values appearing in range (instead of discrete). Consequently, to synthesis 2D ZnO with a single pure phase require great attention during the growth. However, the underlying band gap differences between these 2D ZnO structures open the band gap tunable opportunity (when mixing) to be implemented in optoelectronics via nano-engineering.

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