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Size and strain dependence of electronic properties in ultrathin ZnO nanowires XIHONG PENG, ANDREW COPPLE, QUN WEI, Arizona State University — One dimensional nanostructures of group II-VI semiconductors, in particular ZnO, have drawn broad research interests in recent years due to their potential applications in nano-electronics and nano-optics. In this project, electronic structures of ultrathin wurtzite ZnO nanowires were studied using first-principles Density Functional Theory (DFT) calculations. It was found that the nanowire axial lattice constants shrink compared to that of bulk ZnO. The band gap opens for small nanowires due to the quantum confinement effect. In addition, the band gap can be further tuned using uniaxial strain. The effective masses of the electron and the hole in ZnO can be manipulated not only by the size of nanowire, but also through the applied strain. The results were cross checked using different DFT methods, including GGA, DFT+U, and hybrid functionals.

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