

Abstract Submitted
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First-Principles Optical Cross-Sections of Ultrathin ZnO Nanowires SHELLY ELIZONDO, JOHN MINTMIRE, Oklahoma State University, Department of Physics — One-dimensional nanostructures such as inorganic nanowires and nanotubes represent potential materials for key components of future electronic, optoelectronic, and nanoelectromechanical systems. They will also serve as important model systems to demonstrate quantum-size effects in nanostructured materials. We examine the electronic and optical properties of ZnO nanowires with different geometrical configurations within a first-principles, all-electron self-consistent local density functional (LDF) approach. Orientations along different growth directions are taken into account, with the preferred $\pm [0001]$ direction as the primary focus. The ultrathin nanowires considered here range in diameter from approximately 0.50 nm to 3 nm. We discuss trends in electronic properties and resulting optical properties as a function of nanowire axis orientation and diameter. This work was supported by the US Office of Naval Research, the DoD HPCMO CHSSI program through the Naval Research Laboratory, and the NSF IGERT program.

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