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Electronic and optical properties of InN nanowires from first principles[1] DYLAN BAYERL, EMMANOUIL KIOUPAKIS, University of Michigan Department of Materials Science and Engineering — Group-III-nitride nanowires are promising materials for photovoltaic and solid-state-lighting applications. We use first-principles calculations to investigate the electronic and optical properties of InN nanowires. Density functional theory provides the ground-state properties to which we subsequently apply quasiparticle corrections with the GW method. We thereby accurately predict the electronic band gaps, effective masses, and band dispersions of these nanostructured materials. We further solve the Bethe-Salpeter equation to predict the optical absorption spectra of InN nanowires as a function of cross-sectional dimension and geometry. We demonstrate that quantum confinement can increase the fundamental gap in InN nanowires as high as near-ultraviolet energies.

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