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Electronic and optical properties of two-dimensional GaN from first-principles calculations NOCONA SANDERS, DYLAN BAYERL, GUANG-SHA SHI, EMMANOUIL KIOUPAKIS, Materials Science and Engineering, University of Michigan — GaN is an important commercial semiconductor for solid-state lighting applications (2014 Nobel Prize in Physics). Extreme quantum confinement in atomically thin GaN is a promising method to shift the emission wavelength into the deep ultraviolet range for sterilization applications. Recently, two-dimensional GaN has been experimentally synthesized. We report the electronic and optical properties of two-dimensional GaN using first-principles calculations. We employ density functional theory along with quasiparticle corrections with the GW method to produce accurate band-gap values. We also determine the band structure, carrier effective masses, and optical absorption spectrum. Our results provide microscopic understanding on how the reduction of the thickness to the monolayer regime affects the overall electronic and optical characteristics. This work was supported by the NSF ECCS-CDS&E program under Award No. 1607796. Computational resources were provided by the DOE NERSC facility (DE-AC02-05CH11231).

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