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Electronic and optical properties of atomically thin GaN and InN quantum wells from first principles DYLAN BAYERL, EMMANOUIL KIOUPAKIS, Univ of Michigan - Ann Arbor — Nanostructured group-III-nitrides are of interest for efficient solid-state light emitters in the deep-UV and visible ranges. GaN/AlN and InN/GaN heterostructures with ultrathin GaN or InN layers only a few monolayers thick are especially promising for efficient radiative recombination. We use first-principles calculations to predict the electronic and optical properties of such ultrathin heterostructures and compare to experimental results. Our first-principles approach uses density functional theory plus the GW method to calculate accurate electronic band structures, and the Bethe-Salpeter equation method to predict excitonic properties. We ultimately predict the electronic and optical gaps, exciton binding energies, and radiative lifetimes of GaN/AlN and InN/GaN heterostructures in the ultrathin regime. Our results demonstrate enhancement of excitonic light emission and tunability of the electronic and optical properties in ultrathin III-nitride heterostructures. This work was supported by the NSF DMREF program under Award No. 1534221. Computational resources were provided by the DOE NERSC facility (DE-AC02-05CH11231).

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