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Electronic and optical properties of AlN/GaN superlattices from first-principles calculations DYLAN BAYERL, EMMANOUIL KIOUPAKIS, University of Michigan — Group-III-nitrides are important materials for efficient light emitters in the ultraviolet and visible range. Superlattices of AlN/GaN quantum wells are especially promising for ultraviolet light emission. We use first-principles calculations to investigate the electronic and optical properties of AlN/GaN quantum well superlattices. Density functional theory with quasiparticle corrections from the GW method provides accurate electronic band structures. We then solve the Bethe-Salpeter equation to predict exciton binding energies and fundamental optical emission energies from first principles, yielding good agreement with available experimental measurements. Ultimately, we elucidate the relationship between optical emission energy and well/barrier thickness, as well as demonstrate mitigation of the quantum confined Stark effect in ultra-narrow wells for enhanced radiative recombination efficiency. This research was supported by the J. Robert Beyster Computational Innovation Graduate Fellowship and in part by CSTEC, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science. Computational resources were provided by the DOE NERSC facility.

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