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Accurate treatment of spontaneous polarization in III-nitrides¹ CYRUS E. DREYER, ANDERSON JANOTTI, CHRIS G. VAN DE WALLE, University of California, Santa Barbara — The III-nitride compounds assume the wurtzite crystal structure in the ground state and therefore exhibit spontaneous and piezoelectric dipole moments in the c direction. Discontinuities in these moments at heterostructure interfaces result in electric fields in the layers, which can be detrimental because they separate electrons and holes in quantum wells. Accurate values for polarization differences are critical for understanding and engineering III-nitride heterostructures. Direct experimental measurement of spontaneous polarization has not been possible to date, and calculations are complicated by the necessity to choose a reference structure. The universal choice of reference structure for wurtzite has been zincblende; we demonstrate that this choice does not allow consistent determination of the differences of spontaneous polarizations between materials, which determine their physical manifestation. Using first-principles techniques based on hybrid density functional theory, we have determined polarization discontinuities using a consistent reference based on the hexagonal layered structure of these materials. We will discuss the results in light of available experimental data, and outline consequences for device simulations.

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