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Correct implementation of polarization constants in wurtzite materials and impact on III-nitrides[1] CYRUS E. DREYER, Rutgers University, ANDERSON JANOTTI, University of Deleware , CHRIS G. VAN DE WALLE, University of California, Santa Barbara, DAVID VANDERBILT, Rutgers University — Accurate values for polarization discontinuities between pyroelectric materials are critical for understanding and designing the electronic properties of heterostructures. For wurtzite materials, the zincblende structure has been used in the literature as a reference to determine the effective spontaneous polarization constants. We show that, because the zincblende structure has a nonzero formal polarization, this method results in a spurious contribution to the spontaneous polarization differences between materials. In addition, we address the correct choice of improper versus proper piezoelectric constants. For the technologically important III-nitride materials GaN, AlN, and InN, we determine polarization discontinuities using a consistent reference based on the layered hexagonal structure and the correct choice of piezoelectric constants, [2] and discuss the results in light of available experimental data.

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[2]C. E. Dreyer, A. Janotti, C. G. Van de Walle, and D. Vanderbilt, Phys. Rev. X **6**, 021038 (2016)

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