

Abstract Submitted
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A first-principles study of pyroelectricity in GaN and ZnO JIAN LIU, MARIA V. FERNÁNDEZ-SERRA, PHILIP B. ALLEN, State Univ of NY-Stony Brook — We present first-principles calculations on the primary pyroelectric coefficients for wurtzite GaN and ZnO. The primary pyroelectricity is attributed to the anharmonic atomic displacements of the Born effective charges on the cations and anions. We show that the primary pyroelectricity is the major part of the total pyroelectricity at low temperatures, while the secondary pyroelectricity becomes comparable with the primary pyroelectricity at high temperatures. Our calculations show that contributions from the acoustic and the optical phonon modes to the primary pyroelectric coefficient can be well described by the corresponding Debye and Einstein functions respectively.

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