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Accurate band gaps of AlGaN, InGaN, and AlInN alloys calculations based on LDA-1/2 approach

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We present parameter-free calculations of electronic properties of InGaN, InAlN, and AlGaN alloys. The calculations are based on a generalized quasichemical approach, to account for disorder and composition effects, and first-principles calculations within the density functional theory with the LDA-1/2 approach, to accurately determine the band gaps. We

provide precise results for AlGaN, InGaN, and AlInN band gaps for the entire range of compositions, and their respective bowing parameters.

Topics

Density functional theory, **First-principle calculations**, **Band gap**, **Semiconductors**, **Quasiparticle**, **Metallurgy**, **Photoluminescence spectroscopy**, **Nitrides**, **GW-approximation**

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