Stony Brook University
The Graduate School

Doctoral Defense Announcement

Abstract

A first-principles study of structural, electronic and optical properties of

GaN, ZnO and $(GaN)_{1-x}(ZnO)_x$

By

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GaN and ZnO have spontaneous polarizations comparable with those of ferroelectric materials. Pyroelectricity, namely the temperature dependence of the spontaneous polarization, has not been investigated at the first-principles level. The theory of pyroelectricity is discussed in detail. Through first-principles calculations, I show that anharmonic internal displacement and thermal expansion contribute the major part of the pyroelectricity. An efficient way of calculating third-order force constants at zone-center using the dynamical matrix is proposed.

The semiconductor alloy $(GaN)_{1-x}(ZnO)_x$ shows improved water-splitting efficiency (compared with the pure "end-member" compounds) under visible light illumination. Its main advantage lies in the reduced band gap. We perform Monte-Carlo simulations on a first-principles-based cluster-expansion model to show the existence of short-range order (SRO). We construct the "special quasi-ordered structures" to faithfully include SRO. Subsequent first-principles calculations reveal significant influence of SRO on the structural, electronic and optical properties of $(GaN)_{1-x}(ZnO)_x$ alloy. The role of SRO in the band-gap reduction is explained.

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