Poster Presentation

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First-principles investigation of structural, electronic, optical properties of wurtzite structures

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The second-order susceptibility of crystal determines the intensity of generation of the second optical harmonic. For centrosymmetric crystals, the second-order susceptibility should be zero. One might suggest that reduction of symmetry will lead to some dependence of the second-order susceptibility of crystal on the degree of invariance of crystal structure with respect to inversion η (pseudoinversion). The main goal of our investigation is to answer the question of whether one can use (and to what extent) the quantitative characteristics of pseudoinversion of structures of a number of crystals to describe the structural conditionality of behavior of characteristics of their nonlinear optical properties.

In the present study, structural, electronic, and optical properties of 45 crystals belonging to structural type B4 have been investigated by first-principles calculations using the FP-LAPW method in the framework of density functional theory. The electronic structure and linear optical properties were calculated using both ELK code and WIEN2k code. The nonlinear optical properties were calculated using ELK code. Calculations of the electronic band structure and optical properties were performed using LDA, GGA and mBJ + LDA for exchange–correlation potential. Equilibrium lattice constants a0, c0, bulk modulus B0, first pressure derivative B′ of the bulk modulus, band gaps Eg, symmetry of the valence-to-conduction band transition, dielectric function, second-order nonlinear susceptibility tensor components were obtained. The results obtained for some crystals are in agreement with the well-known experimental and computational data.

A correlation between the second-order nonlinear susceptibility tensor components data arrays and the distributions of crystal structures with respect to their degree of pseudoinversion is analyzed. It is demonstrated that the degree of pseudosymmetry as a quantitative characteristic of crystal structures can be useful for establishing correlations between the structural features of crystals and their physical properties.

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