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Experimental and theoretical investigations of the electronic structure, first and second order optical susceptibilities of BiB3O6 single crystal

Abstract: The first and second order optical susceptibilities of BiB3O6 are calculated using the full potential linear augmented plane wave method. We find that BiB3O6 is a semiconductor with an indirect energy gap of 3.97 eV, to be compared to the experimental value of 4.55 eV. The calculations of the first order optical susceptibilities are compared with our measurements. We present results for the birefringence, and real and imaginary parts of the frequency dependent linear and nonlinear optical response. The calculated birefringence at zero energy is negative, in agreement with our experiments. We calculated and measured the refractive indices, and good agreement is found. Calculations are reported for the frequency dependent complex second order nonlinear optical susceptibilities. BiB3O6 exhibits larger second harmonic generation efficiency than other known materials, such as lithium borate, KTiOPO4, and BaB2O4. Our X-ray photoelectron spectroscopic (XPS) technique measured the concomitant photoemitted electrons with discrete kinetic energies that characterize the emitting atoms and their bonding states. Our XPS measurements show that the BiB3O6 structure contains parallel layers of six-fold coordinated Bi atoms alternating with borate layers, which are constituted by BO4 tetrahedra and BO3 triangles.

Here are some of my publications which are related to the topic of the conference;

9. X-ray photoelectron spectrum measurements and theoretical calculations of the electronic band structure for non-centrosymmetric Bi2ZnB2O7 single crystal. Ali Hussain Reshak, Xuean