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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 BiB_3O_6 are calculated using the full potential linear augmented plane wave method. We find that BiB_3O_6 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. BiB_3O_6 exhibits larger second harmonic generation efficiency than other known materials, such as lithium borate, $KTiOPO_4$, and BaB_2O_4. 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 BiB_3O_6 structure contains parallel layers of six-fold coordinated Bi atoms alternating with borate layers, which are constituted by BO_4 tetrahedra and BO_3 triangles.

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

1. Experimental and theoretical investigation of the First and Second order optical susceptibilities of BiB_3O_6 single crystals, Ali Hussain Reshak , S. Auluck, and I. V. Kityk, Applied Physics A; Materials Science & Processing 91, 451-457 (2008).

2. Linear and Nonlinear optical properties of a novel non centro-symmetric borate oxide $BaBiBO_4$, Ali Hussain Reshak , S. Auluck, and I. V. Kityk, J. Solid State Chemistry 181, 789 (2008).

3. Specific features of second order optical susceptibilities for a complex borate crystal, $Bi_2ZnB_2O_7$: Experiment and theory, Ali H.Reshak, Xuean Chen, I.V. Kityk and S. Auluck, Current Opinion in Solid State & Materials Sciences 11, 33-39 (2007).

4. Energy band structure and density of states for $BaBiBO_4$ non-linear optical crystal, Ali H. Reshak, I.V. Kityk, S. Auluck, J. Alloys compounds 460, 99-102 (2008)

5. X-ray diffraction and optical properties of a non-centrosymmetric borate $CaBiGaB_2O_7$, A H Reshak, Xuean Chen, S. Auluck, I.V. Kityk , J. Chem. Phys. 129, 204111 (2008).

6. Synthesis, IR, UV-VIS spectra, X-ray diffraction and band structure of a non-centrosymmetric borate $CaBiGaB_2O_7$, Ali Hussain Reshak, Xuean Chen, Fangping Song, I.V. Kityk, and S. Auluck, J. Phys. C 21, 205402 (2009).

7. Comparison of the density of states obtained from the X-ray photoelectron spectra with the electronic structure calculations for α-BiB_3O_6 . Ali H. Reshak, S. Auluck, A.Majchrowski, I.V. Kityk, J. J. Appl. Phys. 48, 011601 (2009).

8. X-ray diffraction, crystal structure and spectral features of the optical susceptibilities of single crystals of the ternary borate oxide lead bismuth tetraoxide, $PbBiBO_4$, Ali Hussain Reshak, I.V. Kityk, and S. Auluck, Xuean Chen, J. Phys. Chem. B 113, 6640-6646 (2009) .

9. X-ray photoelectron spectrum measurements and theoretical calculations of the electronic band structure for non-centrosymmetric $Bi_2ZnB_2O_7$ single crystal. Ali Hussain Reshak, Xuean

Chen, I.V. Kityk, S. Auluck, K. Iliopoulos, S. Couris, and R. Khenata, Current Opinion in Solid State & Materials Sciences 12, 26-31 (2009).

10. Influence of the Tm^{+3} concentration on the nonlinear optical effects of the BiB_3O_6:Tm^{+3} glass nanoparticle-doped polymer, A Majchrowski, Jean Ebothe, K Ozga, Ivan V Kityk, Ali Hussain Reshak, T Lukasiewicz and Mikhail G Brik, Journal of Physics D: Applied Physics 43, 015103 (2010)