Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

The structural origin of energy band gap in ultraviolet borates. ZHESHUAI LIN, RAN HE, Technical Institute of Physics and Chemistry, Chinese Academy of Sciences — Borate crystals have been intensively studied for their broad significant application in nonlinear optics materials, fluorescent materials, and laser crystals, especially in the ultraviolet (UV) spectral region (photon energy larger than 6.2 eV). However, due to the structural complexity the mechanism determining the energy band gap in the UV borates still hides in clouds. In this work, the structural origins of the energy band gaps in UV borates are systematically studied by ab initio methods and modeling considerations. Through analyzing the electronic band structures, we find that the top of valence bands in UV borates are dominant from the orbitals on oxygen. These orbitals construct the non-bonding states which determine the energy band gaps and their magnitudes depend on the local environments around oxygen atoms. Accordingly, the UV borates are categorized into three structural types, and in each type the ideal energy band gaps by removing the non-bonding states are almost the same. Moreover, a modified Bond Valence Sum method is adopted to parameterize the local environment around oxygen atoms, and the good agreement between the calculated and experimental energy band gaps within the accuracy of 0.3 eV can be achieved in UV borates.

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Date submitted: 30 Oct 2012 Electronic form version 1.4