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$PbGa_2GeS_6$ crystal as a novel nonlinear optical material: Band structure aspects

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Abstract

New quaternary sulfide $PbGa_2GeS_6$ crystal was synthesized from co-melting high-purity elements The studies of second harmonic generation and the third harmonic generation for new quaternary sulfide $PbGa_2GeS_6$ crystal have shown that its nonlinear optical response is higher with respect to other similar compounds. The band structure analysis performed by X-ray spectroscopy methods and first principles DFT band structure calculations indicate that the main contributions of the S 3p states are located at the top of valence band , while those of the Ga 4p states give contribution to the central and upper portions of the valence band of the $PbGa_2GeS_6$ compound. The calculations reveal that the band gap E_g = 2.445 eV is indirect and is formed between the valence Γ-point and the conduction X-point of Brillouin zone. The theoretically