

Active Performance of Tetrahedral Groups to SHG Response: the Theoretical Interpretations of Ge/Si-Containing Borate crystals

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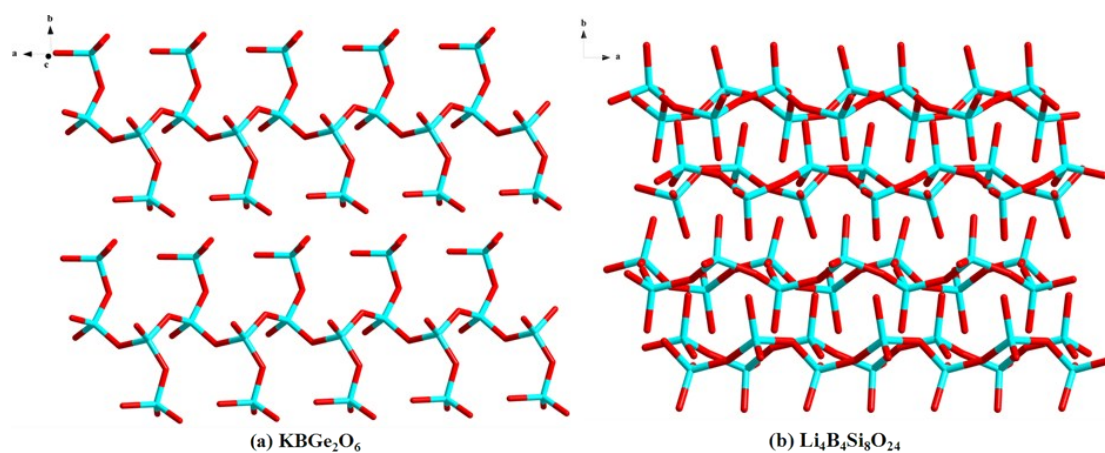


Figure S1. Different R-O patterns of (a) KGe_2O_6 and (b) $\text{Li}_4\text{B}_4\text{Si}_8\text{O}_{24}$.

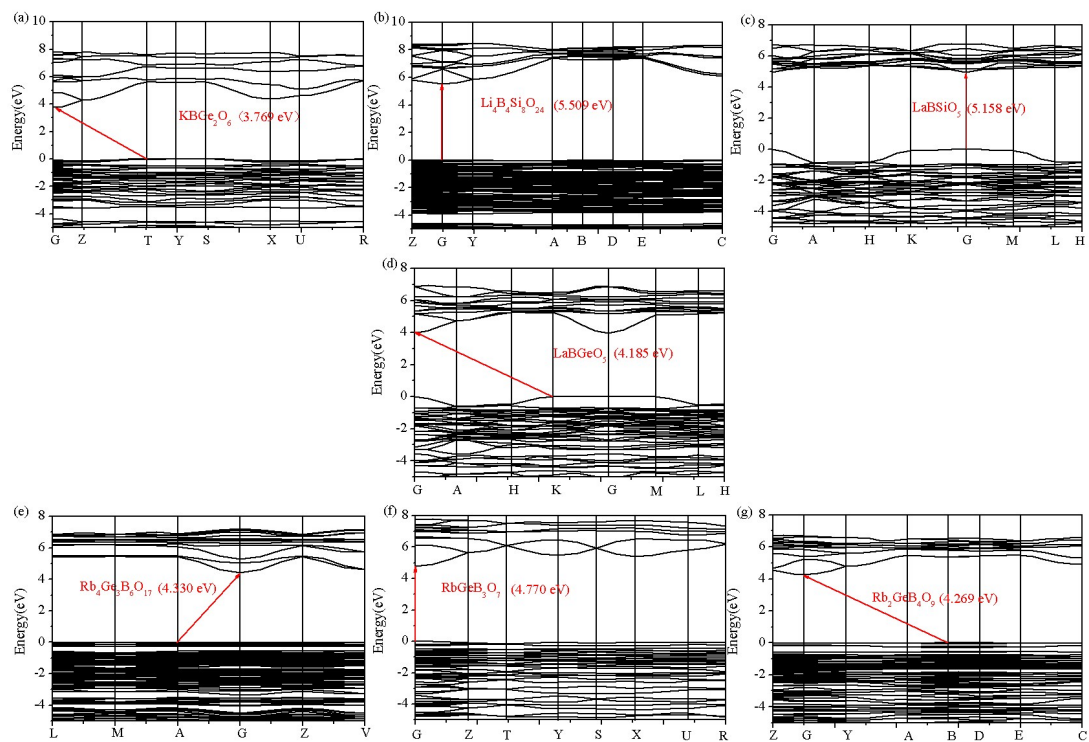


Figure S2. Band structures of KBGe_2O_6 , $\text{Li}_4\text{B}_4\text{Si}_8\text{O}_{24}$, LaBSiO_5 , LaBGeO_5 , $\text{Rb}_4\text{Ge}_3\text{B}_6\text{O}_{17}$, RbGeB_3O_7 and $\text{Rb}_2\text{GeB}_4\text{O}_9$.

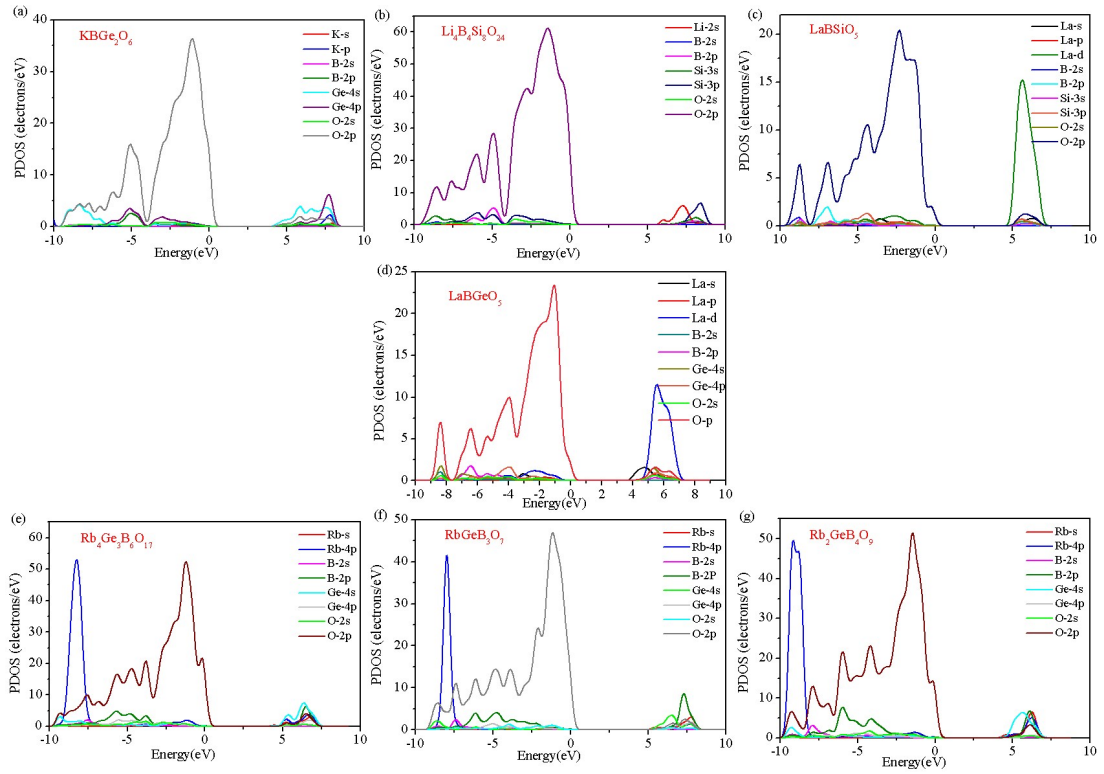


Figure S3. PDOS of KGe_2O_6 , $\text{Li}_4\text{B}_4\text{Si}_8\text{O}_{24}$, LaBSiO_5 , LaGeO_5 , $\text{Rb}_4\text{Ge}_3\text{B}_6\text{O}_{17}$, RbGeB_3O_7 and $\text{Rb}_2\text{GeB}_4\text{O}_9$.