Electronic Supplementary Material (ESI) for RSC Advances.


# Theoretical Perspective of the Lone Pair Activity influencing on Band gap and SHG response in Lead borates

Danni Li[a,b], Qun Jing[a], Chen Lei[a,b], Shilie Pan[a], Bingbing Zhang[a,b], Zhihua Yang[a,*]

[a]*Key Laboratory of Functional Materials and Devices for Special Environments of CAS, Xinjiang Technical Institute of physics & Chemistry of CAS, Xinjiang Key Laboratory of Electronic Information Materials and Devices, 40–1 South Beijing Road, Urumqi 830011, China*

[b] *University of Chinese Academy of Sciences, Beijing 100049,China*

*To whom correspondence should be addressed. E-mail: zhyang@ms.xjb.ac.cn

(Zhihua Yang) Tel: (86)991-3816801; Fax: (86)991-3835096

**Electronic Supplementary Information:**

**The convergence tolerance of $Ba_2[B_5O_9(OH)]\cdot H_2O$ and $Ba_3(B_3O_6)_2$.**

**Figure S1.** The calculated band structure along the high symmetry lines in the Brillouin zone.

**Figure S2.** The convergence tolerance of $Ba_2[B_5O_9(OH)]\cdot H_2O$ and $Ba_3(B_3O_6)_2$.

**Table S1.** The experimental lattice parameters of $Pb_2B_5O_9Cl$, $Ba_2Pb(B_3O_6)_2$, and $BaPb[B_5O_9(OH)]\cdot H_2O$

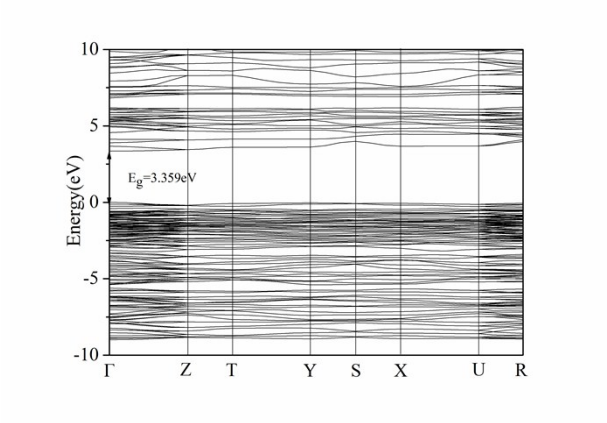
**Table S2.** The optimized parameter of $BaPb[B_5O_9(OH)]\cdot H_2O$ and $Ba_2[B_5O_9(OH)]\cdot H_2O$

**The convergence tolerance of $Ba_2[B_5O_9(OH)]\cdot H_2O$ and $Ba_3(B_3O_6)_2$.**

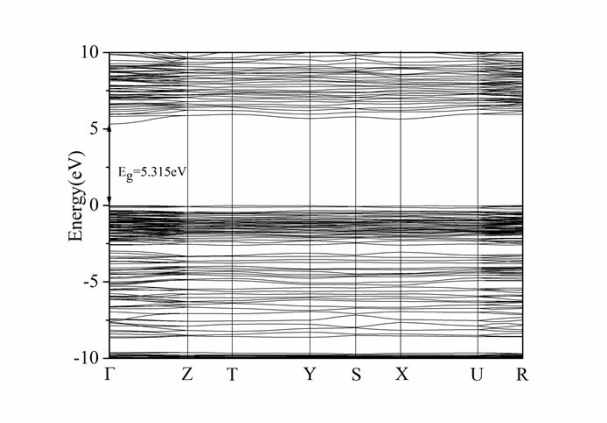
The Energy and Max. displacement of $Ba_2[B_5O_9(OH)]\cdot H_2O$ are $5.0\times10^{-6}$ eV/atom, $5.0\times10^{-4}$ Å. And the Energy and Max. displacement of $Ba_3(B_3O_6)_2$ are $1.0\times10^{-5}$ eV/atom, 0.001 Å.

**Figure S1** The calculated band structure along the high symmetry lines in the Brillouin zone

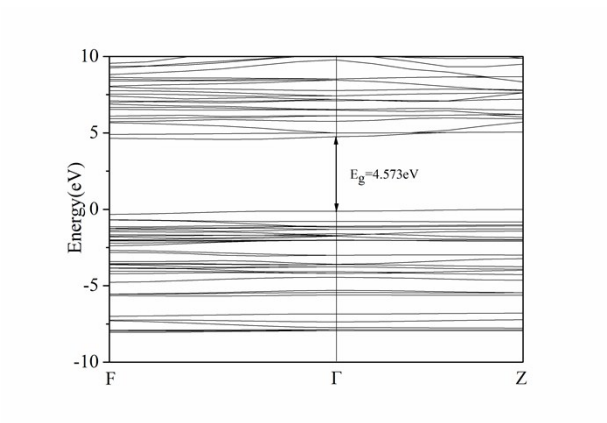
$Pb_2B_5O_9Cl$




$Ba_2B_5O_9Cl$




$Ba_2Pb(B_3O_6)_2$



$Ba_3(B_3O_6)_2$

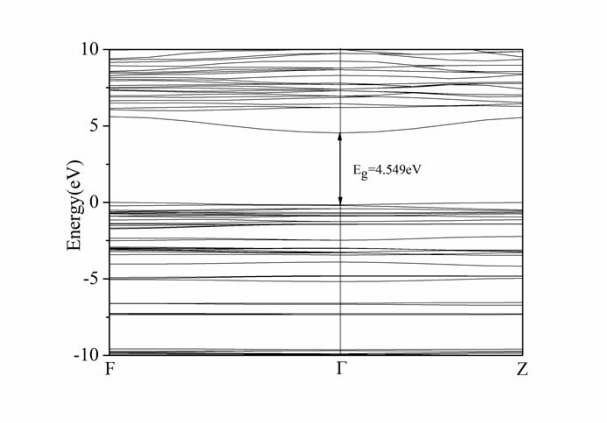


**Table S1** The experimental lattice parameters of $Pb_2B_5O_9Cl$, $Ba_2Pb(B_3O_6)_2$, and $BaPb[B_5O_9(OH)]\cdot H_2O$.

| Compound | a(Å) | b(Å) | c(Å) | α(°) | β(°) | γ(°) |
|---|---|---|---|---|---|---|
| **$Pb_2B_5O_9Cl$** | 11.3543(11) | 11.3629(11) | 6.5535(7) | 90 | 90 | 90 |
| **$Ba_2Pb(B_3O_6)_2$** | 7.2056(8) | 7.2056(8) | 18.752(6) | 90 | 90 | 120 |
| **$BaPb[B_5O_9(OH)]\cdot H_2O$** | 11.3194(6) | 6.6265(3) | 12.9256(8) | 90 | 115.065 | 90 |
| **$Ba_2B_5O_9Cl$** | 11.576(2) | 11.619(9) | 6.6874(13) | 90 | 90 | 90 |

**Table S2** the optimized parameter of compound $BaPb[B_5O_9(OH)]\cdot H_2O$, $Ba_2[B_5O_9(OH)]\cdot H_2O$, and $Ba_3(B_3O_6)_2$.

| compound | a(Å) | b(Å) | c(Å) |
|---|---|---|---|
| **$BaPb[B_5O_9(OH)]\cdot H_2O$** | 11.3194 | 6.6265 | 12.9256 |
| **$Ba_2[B_5O_9(OH)]\cdot H_2O$** | 11.4074 | 6.7225 | 13.3641 |
| **$Ba_3(B_3O_6)_2$** | 7.27809 | 7.27809 | 20.1645 |