Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Two Deep-Ultraviolet Nonlinear Optical Monolayers Obtained by the Template - Optimized Design Strategy

Abudukadi Tudi [a,b], Shujuan Han [a], Zhihua Yang [*a], Shilie Pan [*a]

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

[b]Center of Materials Science and Optoelectronics Engineering, University of Chinese Academy of Sciences, Beijing 100049, China.

To whom correspondence should be addressed :

E-mail: slpan@ms.xjb.ac.cn (Shilie Pan).

E-mail: zhyang@ms.xjb.ac.cn (Zhihua Yang)

Contents

Calculations details

Properties of $B_3O_3F_3$, BOF mono-layer were obtained on the basis of ab initio calculations implemented in the CASTEP package through density functional theory (DFT).[1] The generalized gradient approximation (GGA) [2] was adopted, and Perdew-Burke-Ernzerhof (PBE)[3] functional was chosen to calculate the exchange-correlation potential, with an energy cutoff of 940 eV under the Norm conserving pseudopotentials. The numerical integration of the Brillouin zone was performed using a 4 × 4× 2 Monkhorst-Pack k-point sampling. We set the layer in the xy plane, and adopted a 20 Å supercell length in the z direction to avoid the interaction between the layers.

Table S1. The crystallographic data of BOF

BOF					
*P*3*m*1 (156)					
Cell parameters					
a (Å)	b (Å)	c (Å)	α(°)	β(°)	γ(°)
2.5123	2.5123	21.8567	90	90	120
Fractional coordinates					
Atoms	x	y	z		
B1	0.66667	0.33333	0.02753		
O1	0.33333	0.66667	0.00295		
F1	0.66667	0.33333	0.08820		
Bond lengths (Å)					
B1-O1	1.547	B1-F1	1.326		
Bond valence sum (BVS)					
B1	2.75	O1	1.86	F1	0.89

Table S2. The crystallographic data of $B_3O_3F_3$

$B_3O_3F_3$					
*P*31*m* (157)					
Cell parameters					
a (Å)	b (Å)	c (Å)	α(°)	β(°)	γ(°)
4.2476	4.2476	23.7645	90	90	120
Fractional coordinates					
Atoms	x	y	z		
B1	0.00000	1.00000	-0.61353		
B2	-0.33333	0.33333	-0.65963		
O1	0.00000	0.66387	-0.63650		
F1	0.00000	1.00000	-0.55725		
F2	-0.33333	0.33333	-0.71567		
Bond lengths (Å)					
B1-O1	1.529	B2-O1	1.513		
B1-F1	1.337	B2-F1	1.332		
Bond valence sum (BVS)					
B1	2.82	B2	2.92	O1	2.02
F1	0.86	F2	0.87		

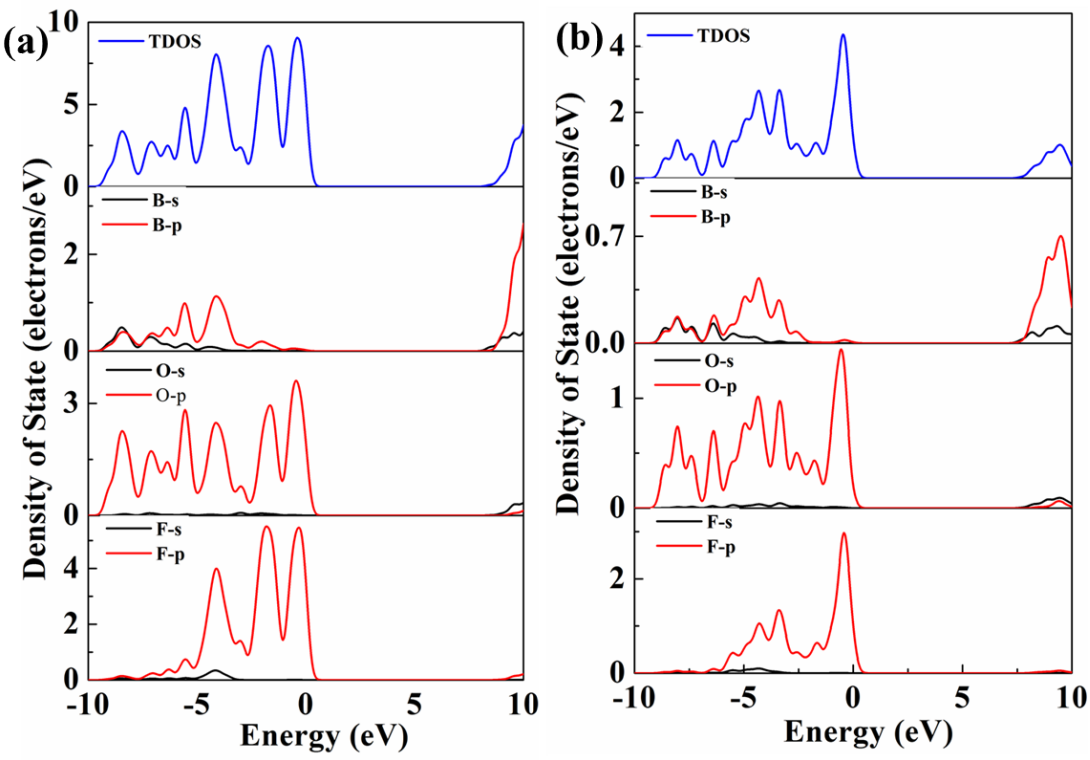

Fig. S1 The PDOS of (a) $B_3O_3F_3$, (b) BOF

References

1 S. J. Clark, M. D. Segall, C. J. Pickard, P. J. Hasnip, M. J. Probert, K. Refson and M. C. Payne, *Z. Kristallogr.,* 2005, **220**, 567.

2 J. P. Perdew, K. Burke and M. Ernzerhof, *Phys. Rev. Lett.,* 1996, 77, 3865.

3 A. M. Rappe, K. M. Rabe, E. Kaxiras and J. D. Joannopoulos, *Phys. Rev. B,* 1990, **41**, 1227.