Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplemental Material for

"Computational Discovery and Characterization of New B_2O Phases"

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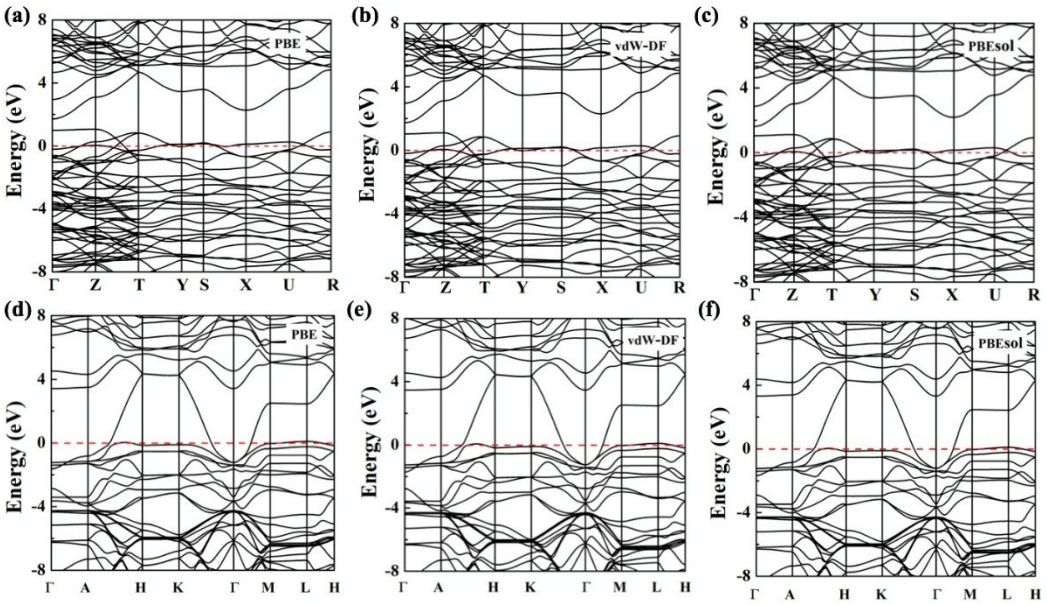

Fig. S1. The calculated electronic band structures for the *Cmmm* phase at 0 GPa (a-c) and *P*-3 phase at 2 GPa (d-f) using the standard PBE-GGA, vdW-DF and PBEsol functionals.

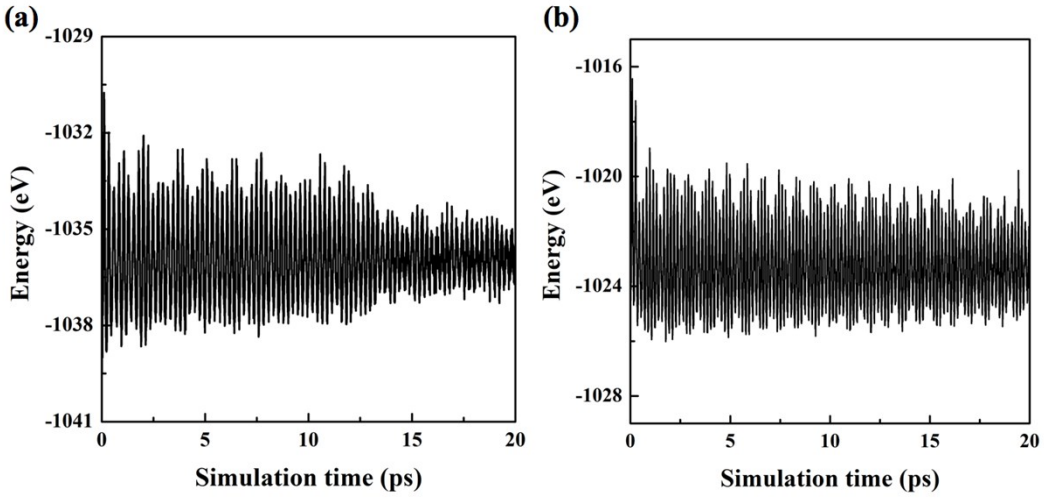

Fig. S2. The fluctuations of the total energy of the *Cmmm* (left) and *P*-3 (right) supercells as a function of the molecular dynamic simulation step at 300 K.

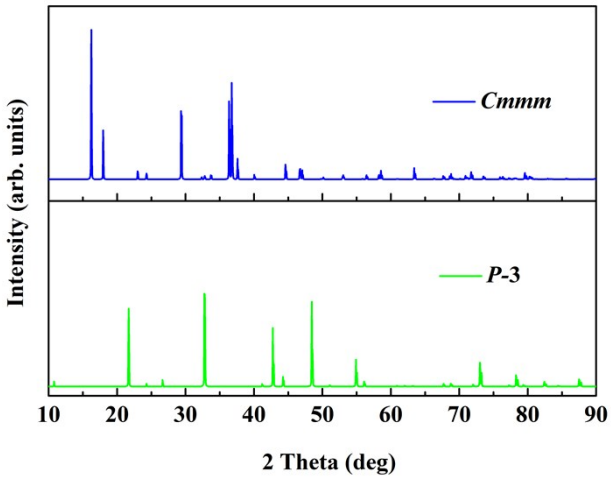

Fig. S3. The simulated X-ray diffraction with λ of 1.5406 Å for the *Cmmm* and *P*-3 phases at 0 and 2 GPa, respectively.

The structural details (in cif format) of the two newly predicted B_2O phases.

For *Cmmm* at 0 GPa:

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_pd_phase_name                          ''
_cell_length_a                          5.53300
_cell_length_b                          10.90600
_cell_length_c                          5.46600
_cell_angle_alpha                       90
_cell_angle_beta                        90
_cell_angle_gamma                       90
_symmetry_space_group_name_H-M          'C m m m'
_symmetry_Int_Tables_number             65

loop_
_symmetry_equiv_pos_as_xyz
   'x, y, z'
   '-x, -y, -z'
   '-x, -y, z'
   'x, y, -z'
   '-x, y, -z'
   'x, -y, z'
   'x, -y, -z'
   '-x, y, z'
   'x+1/2, y+1/2, z'
   '-x+1/2, -y+1/2, -z'
   '-x+1/2, -y+1/2, z'
   'x+1/2, y+1/2, -z'
   '-x+1/2, y+1/2, -z'
   'x+1/2, -y+1/2, z'
   'x+1/2, -y+1/2, -z'
   '-x+1/2, y+1/2, z'

loop_
   _atom_site_label
   _atom_site_occupancy
   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_adp_type
   _atom_site_U_iso_or_equiv
   _atom_site_type_symbol
   B1     1.0     0.342200     0.635700     0.500000     Uiso   1.000000 B
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B2	1.0	0.228300	0.500000	0.334700	Uiso	1.000000	B
B3	1.0	0.500000	0.580800	0.779600	Uiso	1.000000	B
O4	1.0	0.000000	0.852500	0.000000	Uiso	1.000000	O
O5	1.0	0.250000	0.750000	0.500000	Uiso	1.000000	O
O6	1.0	0.000000	0.500000	0.769300	Uiso	1.000000	O

For *P*-3 at 2 GPa

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_pd_phase_name                          ''
_cell_length_a                          4.18900
_cell_length_b                          4.18900
_cell_length_c                          7.95600
_cell_angle_alpha                       90
_cell_angle_beta                        90
_cell_angle_gamma                       120
_symmetry_space_group_name_H-M          'P -3'
_symmetry_Int_Tables_number             147

loop_
_symmetry_equiv_pos_as_xyz
   'x, y, z'
   '-x, -y, -z'
   '-y, x-y, z'
   'y, -x+y, -z'
   '-x+y, -x, z'
   'x-y, x, -z'

loop_
   _atom_site_label
   _atom_site_occupancy
   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_adp_type
   _atom_site_U_iso_or_equiv
   _atom_site_type_symbol
   B1    1.0    0.004500    0.670200    0.775300    Uiso    1.000000 B
   B2    1.0    0.097100    0.691200    0.561000    Uiso    1.000000 B
   O3    1.0    0.335300    0.005000    0.846200    Uiso    1.000000 O
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