

SUPPORTING INFORMATION FOR:

Selected-Control Hydrothermal Growths of α - and β - PbO Crystals and Oriented Pressure Induced Phase Transition

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1, Details of the DFT calculation:

Density of states (DOS) calculations were performed using a first-principles plane-wave pseudopotential method based on density functional theory with CASTEP package,¹ and the ion-electron interactions were modeled by the ultrasoft pseudopotentials.² Norm-conserving pseudopotentials are adopted with an energy cutoff of 900 eV. K meshes with a density of 0.02 Å⁻¹ are adopted. Other calculating parameters and convergent criterions were set by the default values of CASTEP code. Unit cell parameters and atomic coordinates of α - and β - PbO from ICSD-94333 (*P4/nmms*) and ICSD-60135 (*Pbcm*) are adopted as initial structure model. The operation of antistrophic pressures are simulated by varying the interlayer distances of adjacent rock-salt-like blocks, while the bond lengths and bond angles of PbO₄ within the layer are fixed. The interlayer distances (*c* of α -PbO, *a* of β -PbO), corresponding atom coordinations and E-E⁰ are listed in the follows:

<i>c</i> of α -PbO	<i>z</i> of Pb	E-E ⁰	<i>a</i> of β -PbO	<i>x</i> of Pb	<i>x</i> of O	E-E ⁰
4.1	0.29219	1.37178	4.1	0.33016	-0.19361	13.03599
4.2	0.28523	1.09645	4.2	0.32230	-0.18900	10.30199
4.3	0.27860	0.86009	4.3	0.31480	-0.18460	8.15456
4.4	0.27226	0.65722	4.4	0.30765	-0.18041	6.46627
4.5	0.26621	0.49359	4.5	0.30081	-0.17640	5.12579
4.6	0.26043	0.34828	4.6	0.29427	-0.17257	4.05893
4.7	0.25489	0.22771	4.7	0.28801	-0.16889	3.20385
4.8	0.24958	0.15733	4.8	0.28201	-0.16538	2.51899
4.9	0.24448	0.07981	4.9	0.27625	-0.16200	1.96985
5.0227	0.23851	-2.046E-6	5.0	0.27073	-0.15876	1.53373
5.1	0.23489	-0.04370	5.1	0.26542	-0.15565	1.18588
5.2	0.23038	-0.04098	5.2	0.26032	-0.15265	0.91410
5.3	0.22603	-0.06664	5.3	0.25540	-0.14977	0.69600
5.4	0.22185	-0.08591	5.4	0.25068	-0.14700	0.52914
5.5	0.21781	-0.10092	5.5	0.24612	-0.14433	0.40005
5.6	0.21392	-0.11052	5.6	0.24172	-0.14175	0.30520
5.7	0.21017	-0.11856	5.7	0.23748	-0.13926	0.23664
5.8	0.20655	-0.10423	5.8	0.23339	-0.13686	0.17825
5.9	0.20304	-0.10924	5.8931	0.22970	-0.13470	0.14116
6.0	0.19966	-0.11072	6.0	0.22561	-0.13230	0.11297
6.1	0.19639	-0.08299	6.1	0.22191	-0.13013	0.10201
6.2	0.19322	-0.07924	6.2	0.21833	-0.12803	0.08850
6.3	0.19015	-0.07469	6.3	0.21486	-0.12600	0.07900
6.4	0.18718	-0.07138	6.4	0.21151	-0.12403	0.07314
6.5	0.18430	-0.07108	6.5	0.20825	-0.12212	0.07046

Reference:

(1) S. J. Clark, M. D. Segall, C. J. Pickard, P. J. Hasnip, M. J. Probert, K. Refson, M. C. Payne, *Z. Kristallogr.*, 2005, **220**, 567.
(2) D. Vanderbilt, *Phys. Rev. B*, 1990, **41**, 7892.

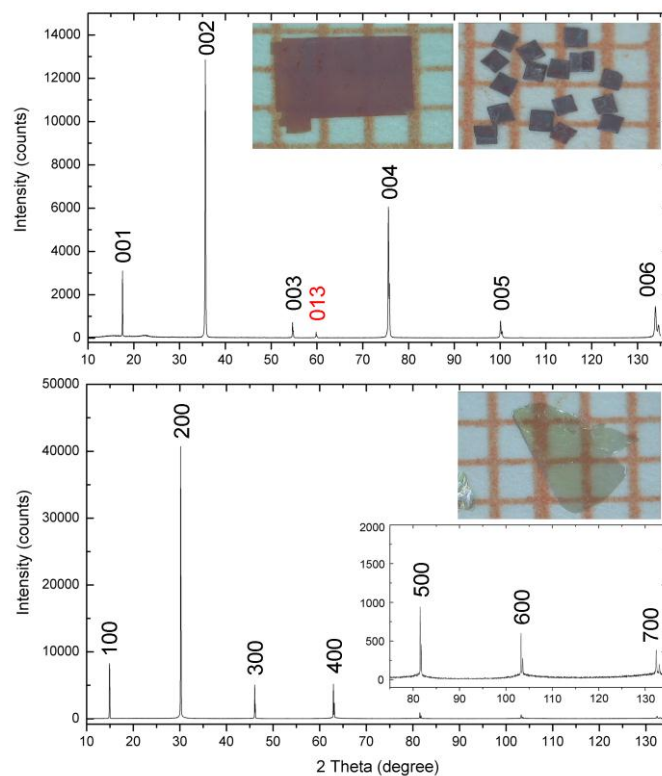


Figure S1. X-ray diffraction pattern of α - (up) and β - (down) PbO single crystals along the direction of the sheets. Insert shows the images of the as-grown crystals.

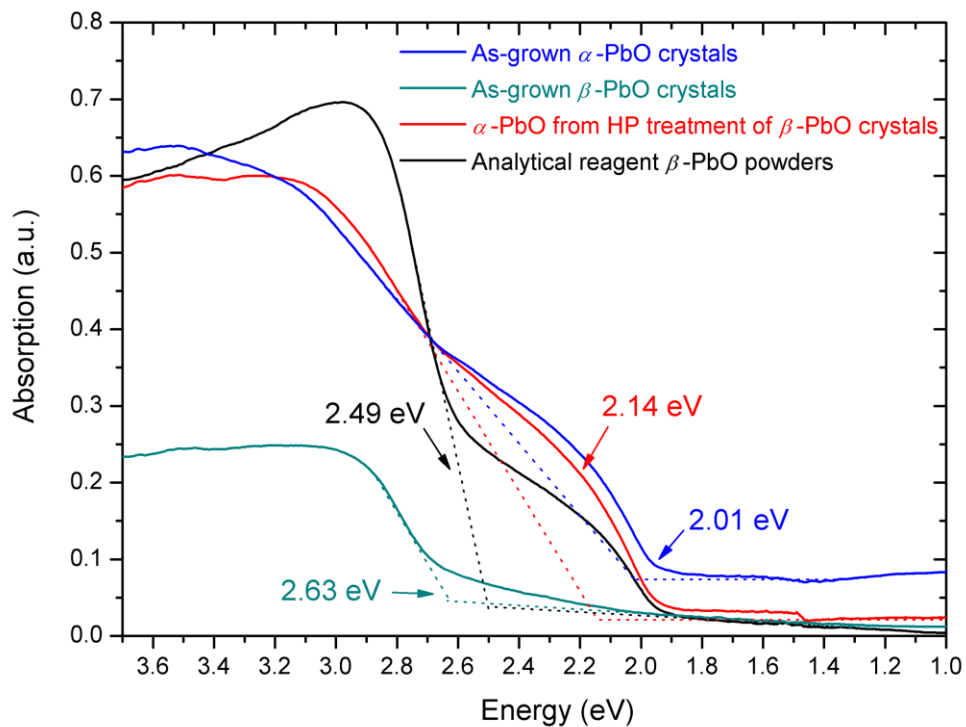


Figure S2. UV-visible absorption spectra of as-grown α - and β - PbO single crystals, α - PbO powders obtained from phase transition of β - PbO crystals, and commercial analytical pure β - PbO reagent.

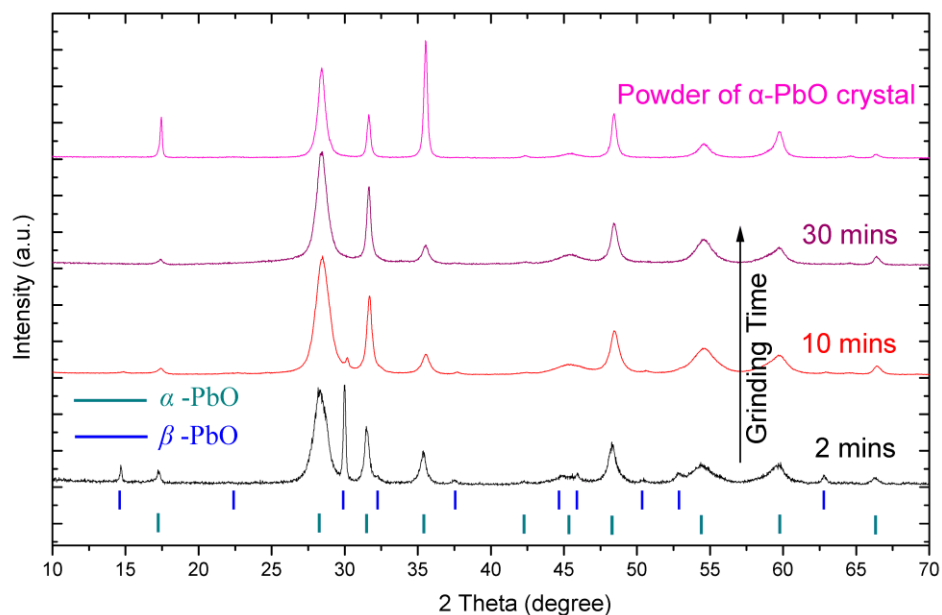


Figure S3. X-ray diffraction patterns of β -PbO crystal as a function of grinding time. The short vertical bars represent the theoretical Bragg reflection positions of α - and β -PbO, respectively.

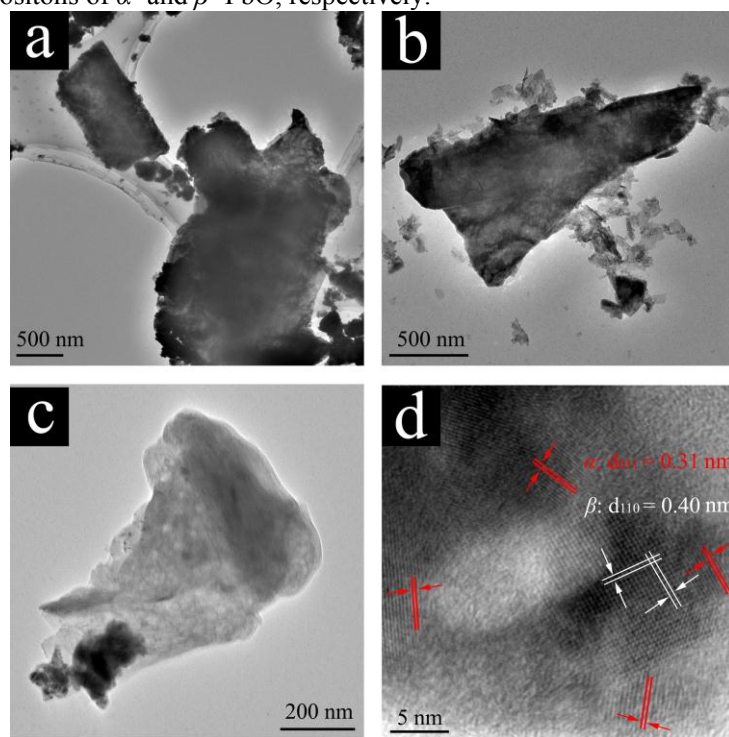


Figure S4. TEM images of α -PbO (a) and β -PbO (b, c) crystal sheets. (d), HRTEM image of β -PbO after being treated by pressure perpendicular to the crystal sheet.