Supporting Information for

High Mechanical Strength in $Zn_4B_6O_{13}$ with Unique Sodalite-cage Structure

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Figure S1 The XRD patterns at ambient condition of ZBO collected by laboratory XRD facility with Cu radiation .

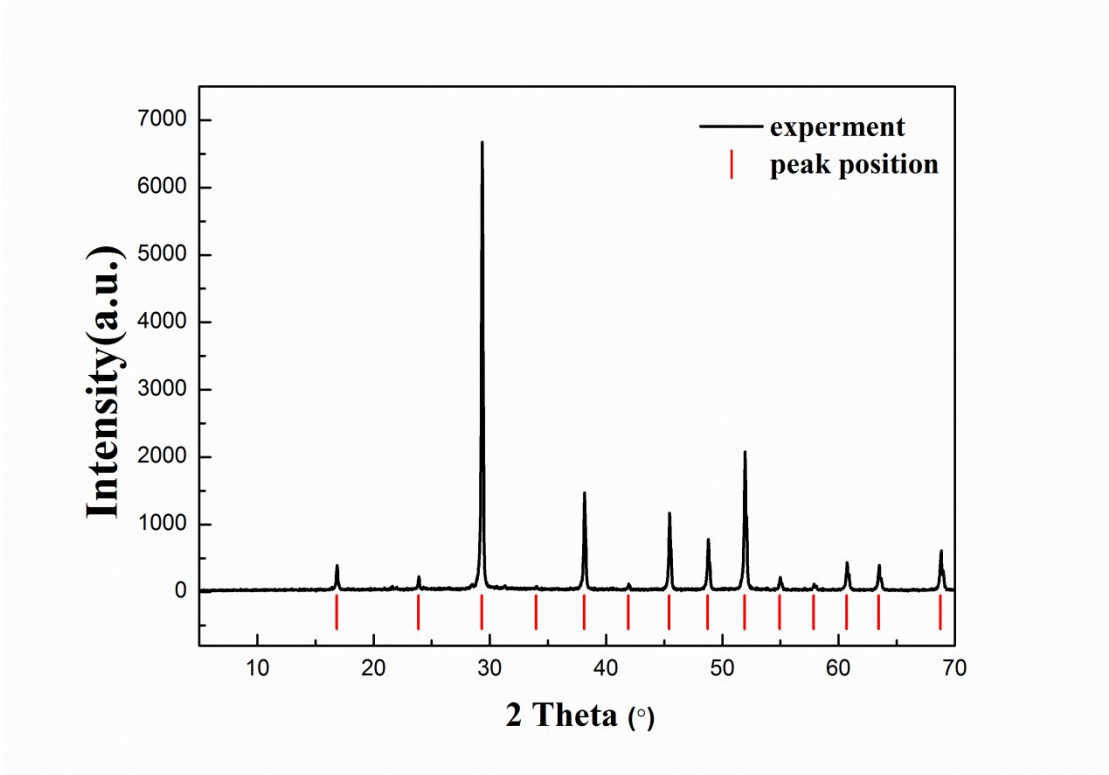

Figure S2 The diffractograms of ZBO at various pressure.

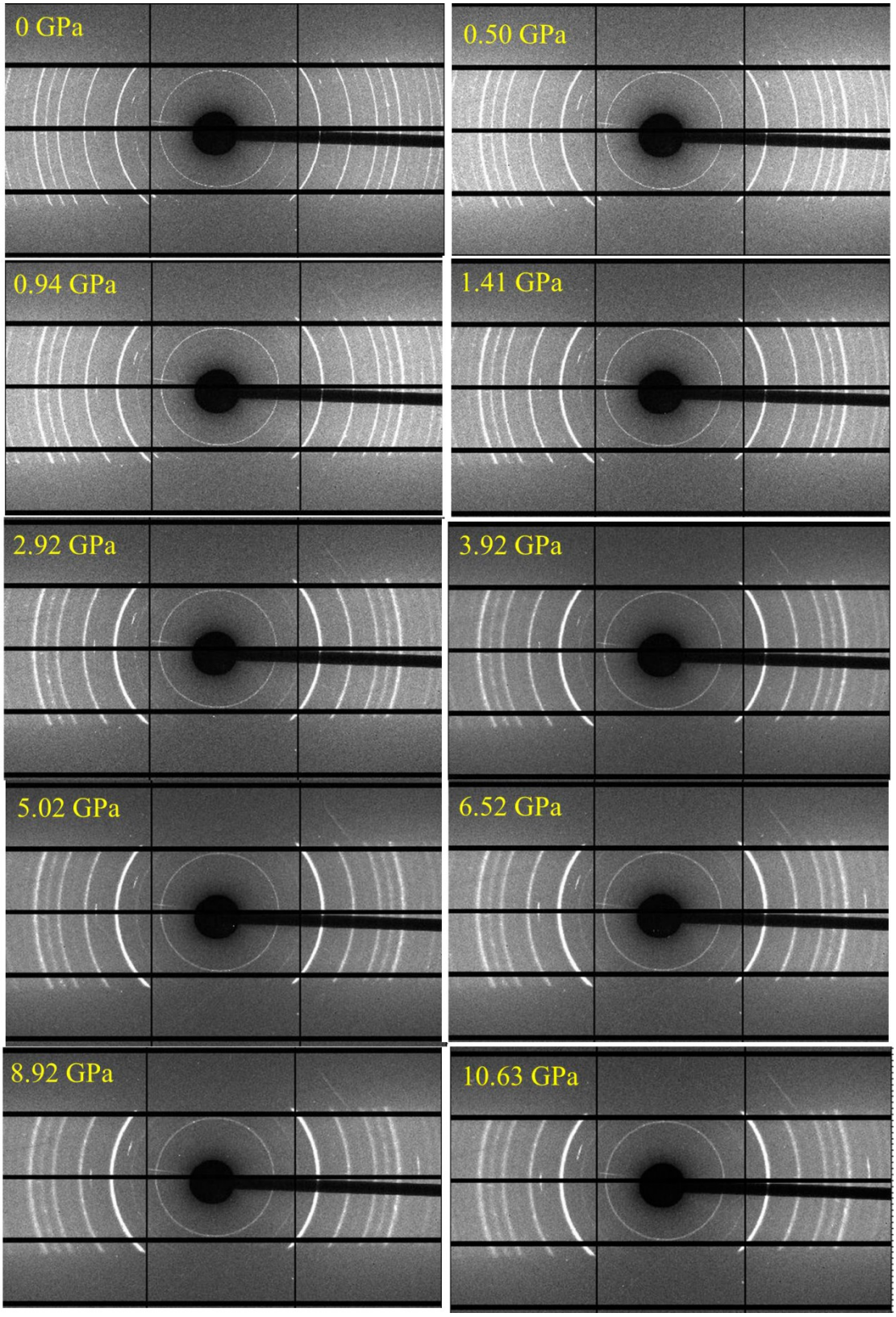

Figure S3 The high pressure X-ray diffraction patterns of ZBO

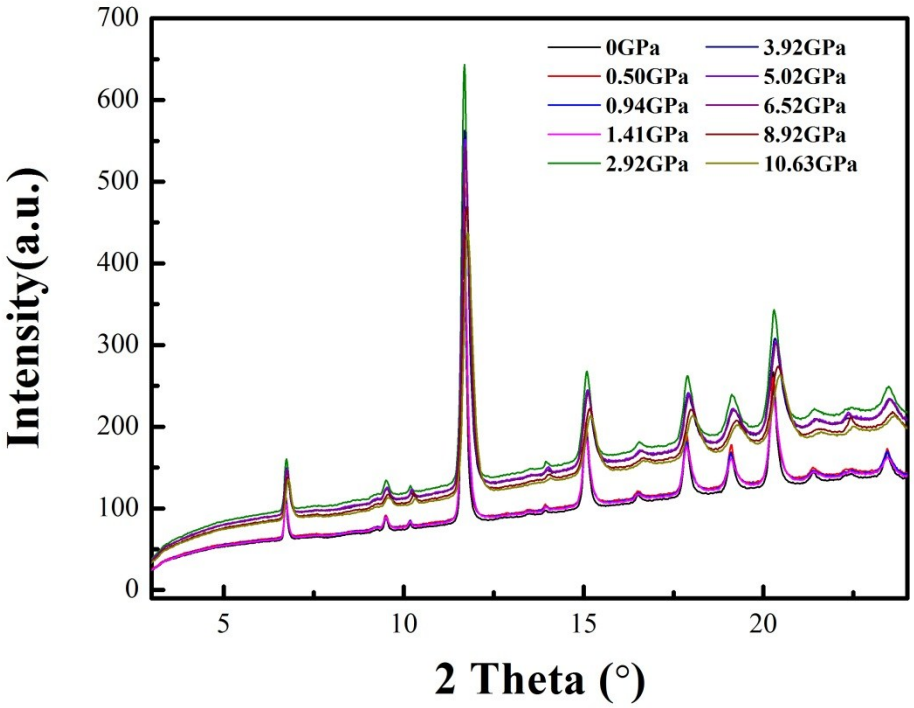

Figure S4 Refinement plots for XRD patterns at (a) 0 GPa and (b) 10.63 GPa of ZBO. The observed (×), calculated (red solid line), and difference profiles (blue solid line) are shown along with the reflection positions (magenta vertical bars)

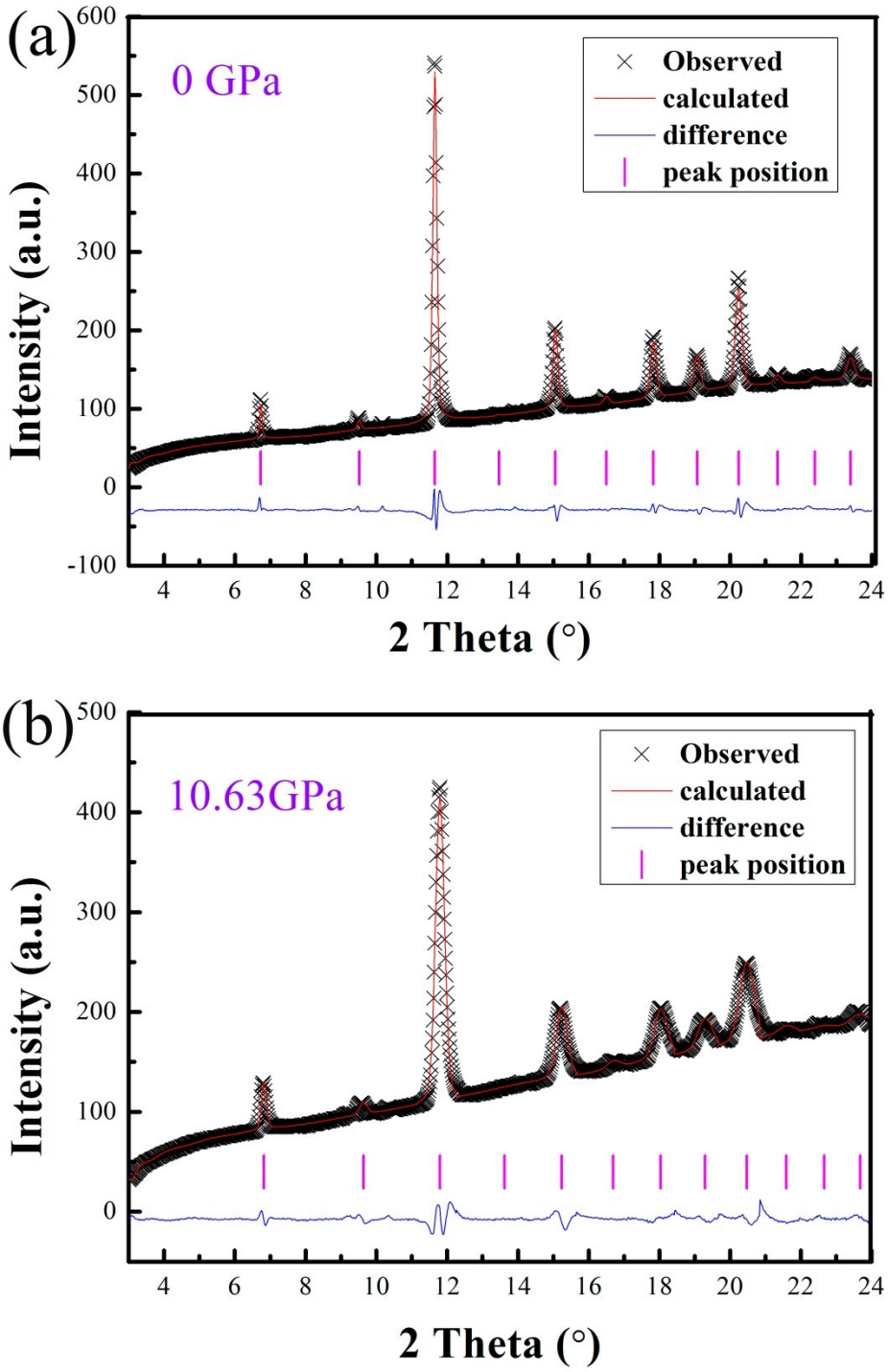

Figure S5 Density of states of ZBO at various pressure. (a) the density of states and partial density of states at 0GPa (b) the density of states of Zn and O atom under 0GPa and 10.63GPa. It is clear that the electronic energy levels near the top of valence band (VB) and the bottom of conduction band (CB) are dominantly composed of the zinc and oxygen orbitals, indicating that the band gap of ZBO is determined mainly by the electron transition within the Zn–O bonds. As pressure increase from 0 to 10.63GPa, the contraction of Zn-O bonds reinforces the hybridization between zinc and oxygen atoms, which lower the energy of the electron states at the top of VB. Thus it requires crossing wider energy range for electrons to transit from VB to CB, so the band gap is broadened.

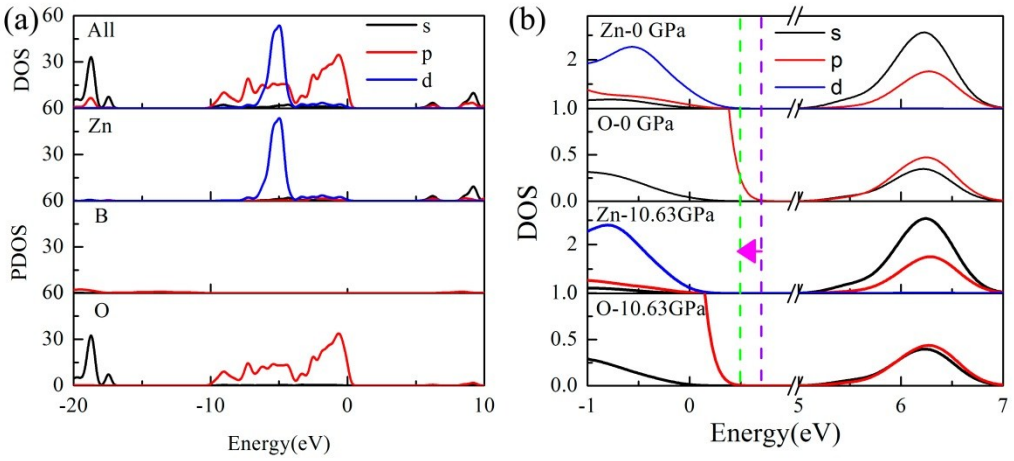

Table S1 Lattice parameters of ZBO at various pressure

Pressure(GPa)	Lattice parameter(Å)
0	7.4957(7)
0.50	7.4741(9)
0.94	7.4690(1)
1.41	7.4584(3)
2.92	7.4414(3)
3.92	7.4354(3)
5.02	7.4180(3)
6.52	7.4161(3)
8.92	7.4024(4)
10.63	7.3881(4)

Table S2 The B-O bond, Zn-O2 bond and ∠B-O-B angle at various pressure

Pressure (GPa)	B-O bond(Å)	Relative value	Zn-O2 bond(Å)	Relative value	∠B-O-B(°)	Relative value
0	1.472	1.000	1.979	1.000	128.301	1.000
0.50	1.470	0.999	1.972	0.996	128.068	0.998
0.94	1.469	0.998	1.971	0.996	128.048	0.998
1.41	1.468	0.997	1.968	0.994	127.843	0.996
2.92	1.465	0.995	1.963	0.992	127.745	0.996
3.92	1.464	0.994	1.961	0.991	127.718	0.995
5.02	1.462	0.993	1.956	0.988	127.587	0.994
6.52	1.461	0.993	1.956	0.988	127.560	0.994
8.92	1.459	0.991	1.952	0.986	127.447	0.993
10.63	1.457	0.990	1.948	0.984	127.346	0.993

Table S3 The bandgap at various pressure

Pressure(GPa)	Eg (eV)	UV absorption edge(nm)
0	5.341	232.2
0.50	5.401	229.6
0.94	5.407	229.3
1.41	5.426	228.5
2.92	5.463	227.0
3.92	5.475	226.5
5.02	5.512	225.0
6.52	5.513	224.9
8.92	5.538	223.9
10.63	5.566	222.8

Table S4 The CCDC number of the CIF files under different pressure

CIF files	CCDC
$Zn_4B_6O_{13}$_0	1519591
$Zn_4B_6O_{13}$_0.50	1519593
$Zn_4B_6O_{13}$_0.94	1519594
$Zn_4B_6O_{13}$_1.41	1519595
$Zn_4B_6O_{13}$_2.92	1519596
$Zn_4B_6O_{13}$_3.92	1519597
$Zn_4B_6O_{13}$_5.02	1519598
$Zn_4B_6O_{13}$_6.52	1519599
$Zn_4B_6O_{13}$_8.92	1519600
$Zn_4B_6O_{13}$_10.63	1519592