

Supplementary Material of

Joint experimental and theoretical study of bulk Y₂O₃ at high pressure

A.L.J. Pereira^{1,2*}, J.A. Sans¹, O. Gomis³, D. Santamaría-Pérez⁴, S. Ray⁵, A. Godoy-Jr.², A. S. da Silva-Sobrinho², P. Rodríguez-Hernández⁶, A. Muñoz⁶, C. Popescu⁷ and F. J. Manjón^{1*}

¹ *Instituto de Diseño para la Fabricación y Producción Automatizada, MALTA Consolider Team,
Universitat Politècnica de València, 46022 València, Spain*

² *Laboratório de Plasmas e Processos – LPP, Instituto Tecnológico de Aeronáutica – ITA, 12228-900
São José dos Campos, Brazil*

³ *Centro de Tecnologías Físicas, MALTA Consolider Team, Universitat Politècnica de València,
46022 Valencia, Spain*

⁴ *Departament de Física Aplicada-ICMUV, MALTA Consolider Team, Universitat de Valencia,
Burjassot, Spain*

⁵ *Department of Chemistry, AISECT University, Bhopal, India*

⁶ *Departamento de Física, Instituto de Materiales y Nanotecnología, MALTA Consolider Team,
Universidad de La Laguna, 38207 San Cristóbal de La Laguna, Spain*

⁷ *ALBA-CELLS, MALTA Consolider Team, 08290 Cerdanyola del Vallès (Barcelona), Catalonia,
Spain*

*Corresponding authors: A.L.J. Pereira (andreljp@ita.br), F.J. Manjón (fjmanjon@fis.upv.es)

Table S1. Lattice parameters and atomic coordinates of Y_2O_3 polymorphs obtained by our theoretical calculations at selected pressures.

Cubic (Ia-3, SG 206, C-type) 1 atm			Trigonal (P-3m1, SG 164, A-type) 15.9 GPa			Monoclinic (C12/m1, SG 12, B-type) 1 atm		
Lattice Parameters								
a (Å)	10.59105		3.65504			13.89853		
b (Å)	-		-			3.48560		
c (Å)	-		5.80550			8.59999		
β (°)	-		-			100.15985		
Atomic Positions								
x	y	z	x	y	z	x	y	z
Y1 – 8a			Y1 – 2d			Y1 – 4i		
0	0	0	0.33333	0.66666	0.24845	0.13530	0	0.48693
Y2 – 24d			O1 – 1a			Y2 – 4i		
0.28282	0	0.25	0	0	0	0.19041	0	0.13707
O1 – 48e			O2 – 2d			Y3 – 4i		
0.35921	0.87022	0.40456	0.33333	0.66666	0.64651	0.46719	0	0.18675
			O1 – 4i					
						0.62830	0	0.28264
			O2 – 4i					
						0.32529	0	0.02996
			O3 – 4i					
						0.29338	0	0.37651
			O4 – 4i					
						0.02842	0	0.65633
			O5 – 2a					
						0	0	0

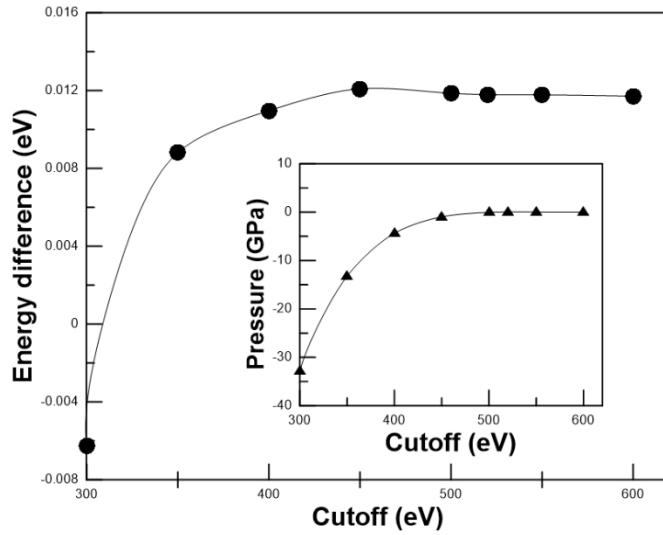


Figure S1. Total energy difference between two selected volumes as function of cutoff energy. Inset shows the isotropic pressure for a selected volume as a function of cutoff energy.

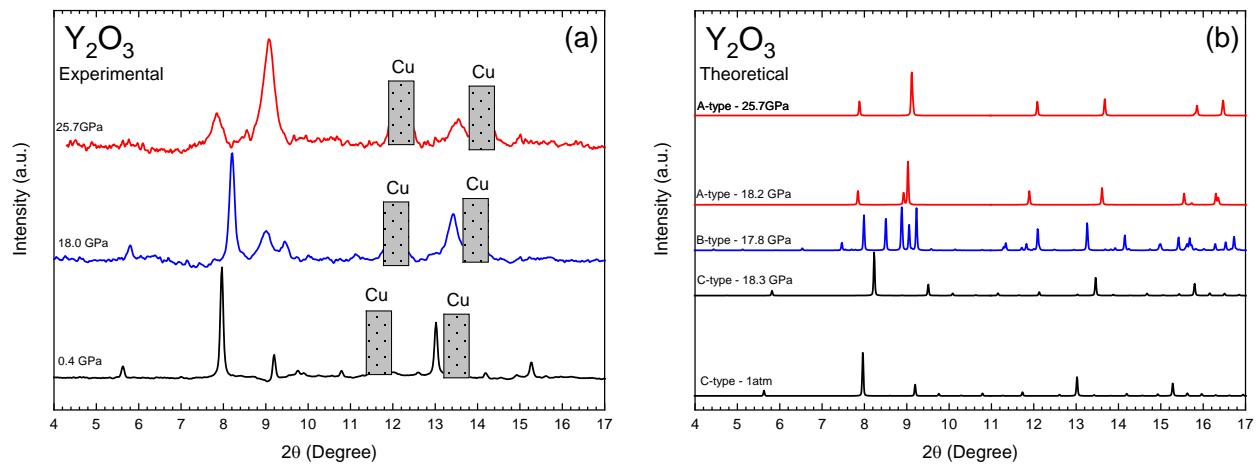


Figure S2. (a) Experimental and (b) theoretical XRD pattern of Y_2O_3 at different pressures. The C-, B- and A-type theoretical patterns were obtained from crystalline structures optimized through theoretical calculations at different pressures.

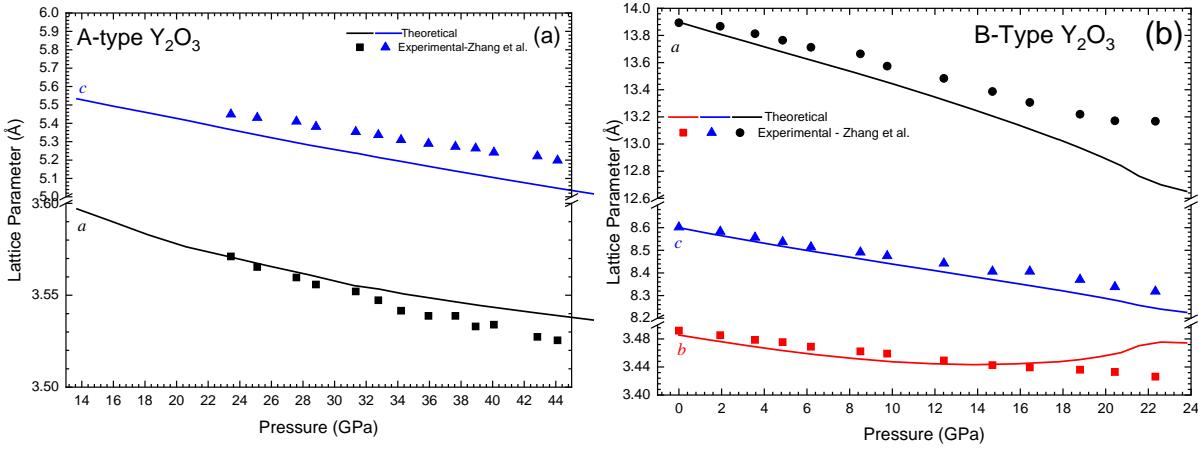


Figure S3. Theoretical pressure dependence of the lattice parameters of A-type Y_2O_3 (a) and B-type Y_2O_3 (b). Experimental data are from Zhang et al. [S1].

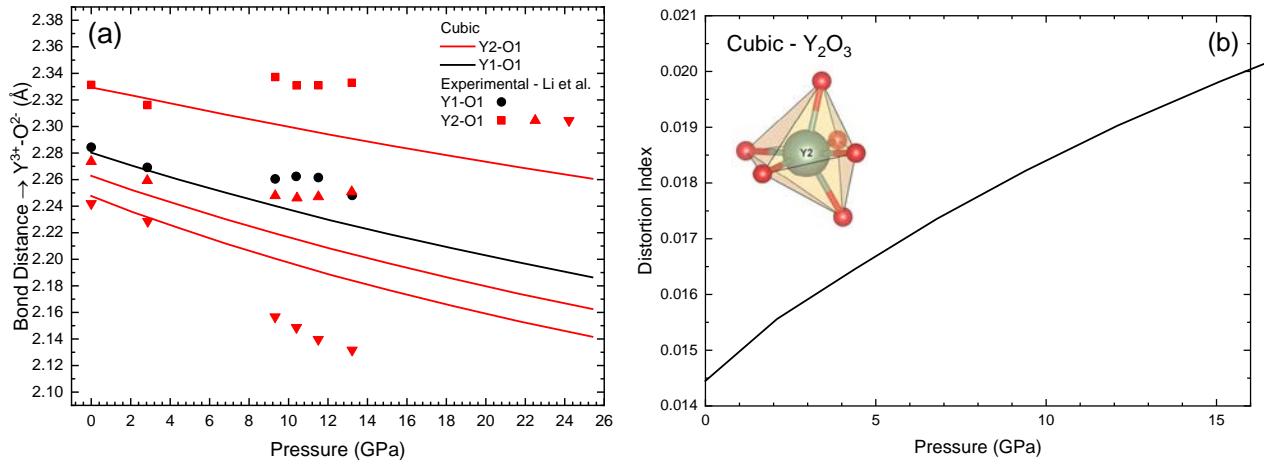


Figure S4. Theoretical pressure dependence of the (a) Y-O distance and (b) distortion of the Y_2 octahedron in C-type bulk Y_2O_3 . Experimental data for bulk $\text{Y}_2\text{O}_3:\text{Eu}^{3+}$ nanotubes from Li et al. [S2] have been added for comparison.

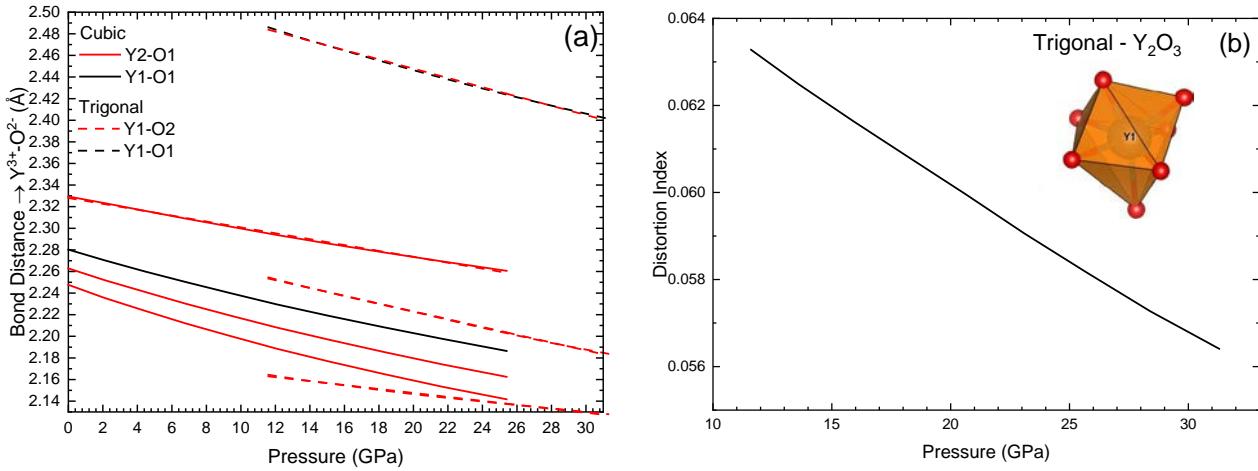


Figure S5. Theoretical pressure dependence of the (a) Y-O distance and (b) distortion of the Y1 polyhedral units in A-type bulk Y_2O_3 . In order to facilitate the comparison with C-type Y_2O_3 , the evolution of the Y-O distances for C-type bulk Y_2O_3 is added in (a).

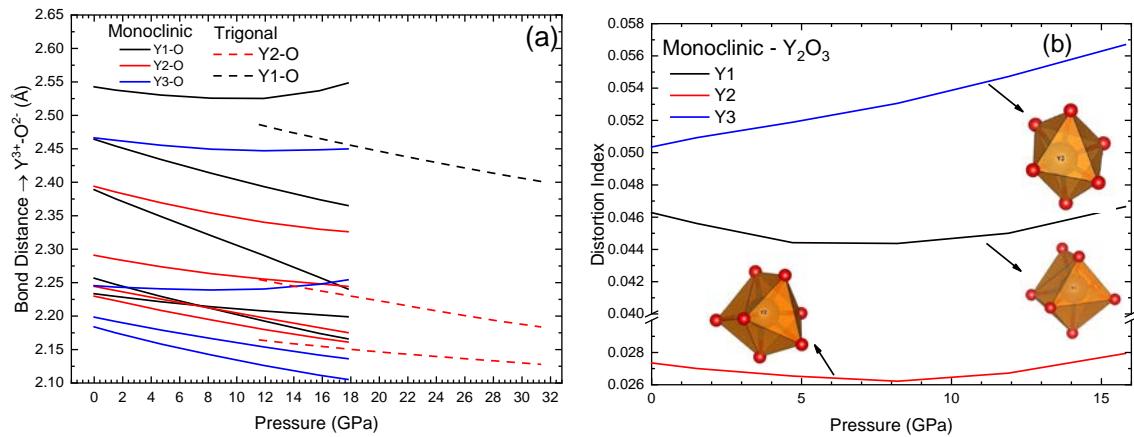


Figure S6. Theoretical pressure dependence of the (a) Y-O distance and (b) distortion of the Y1, Y2 and Y3 polyhedral units in B-type bulk Y_2O_3 . In order to facilitate the comparison, in (a) we added the evolution of the Y-O distances for A-type bulk Y_2O_3 .

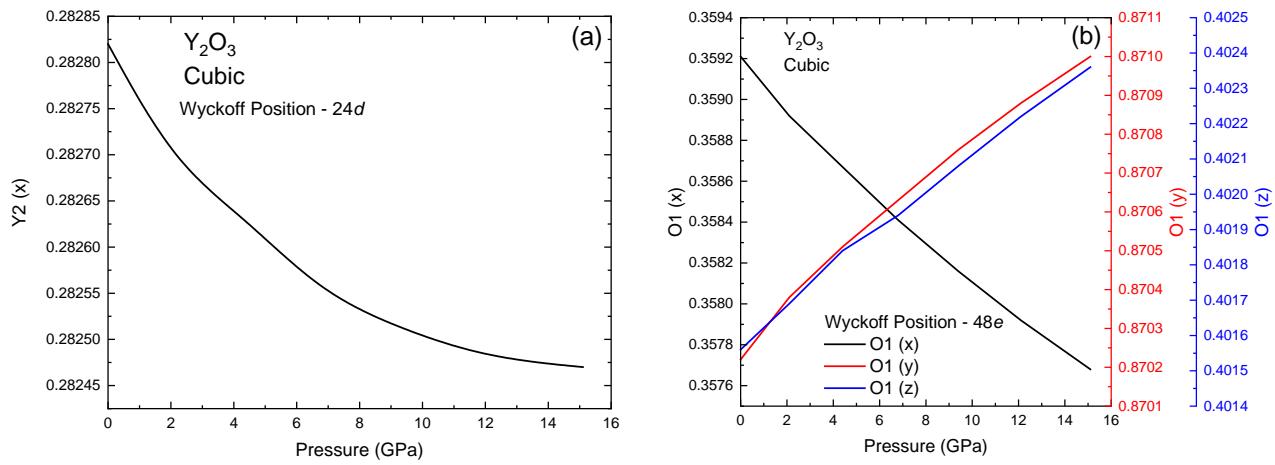


Figure S7. Theoretical pressure dependence of the free Wyckoff position of (a) Y2 and (b) O1 atoms in C-type Y_2O_3 .

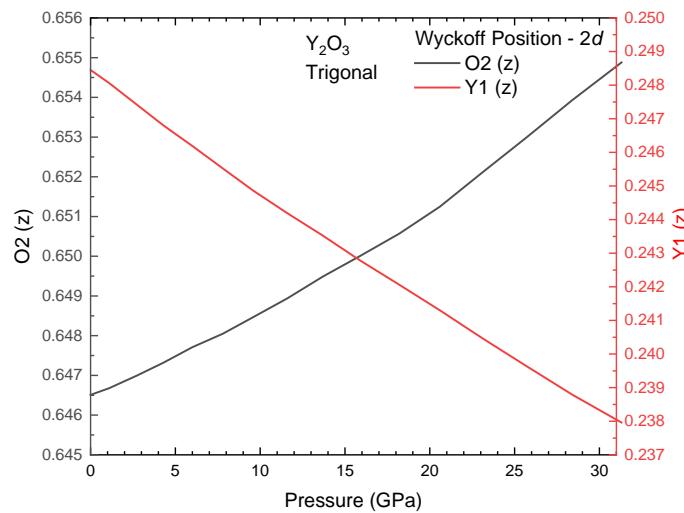


Figure S8. Theoretical pressure dependence of the free Wyckoff positions of Y1 and O2 atoms in A-type Y_2O_3 .

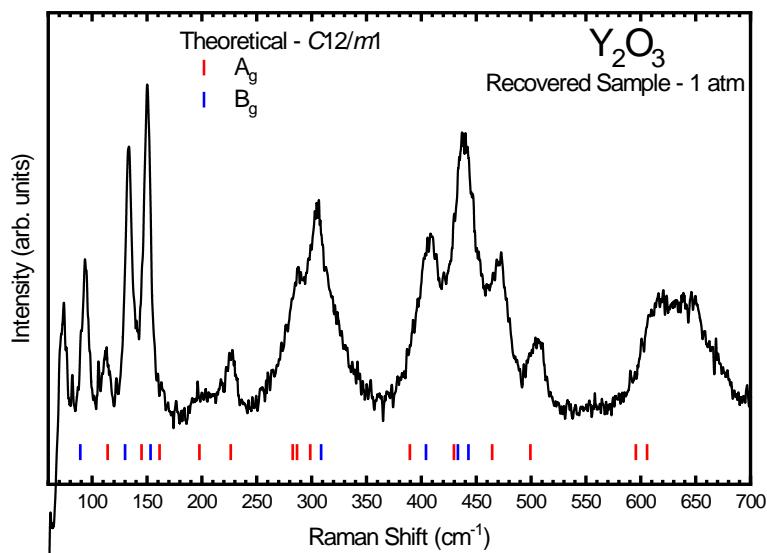


Figure S9. Raman spectrum of bulk B-type Y_2O_3 at room conditions. Bottom marks indicate the frequencies of the theoretical Raman-active modes.

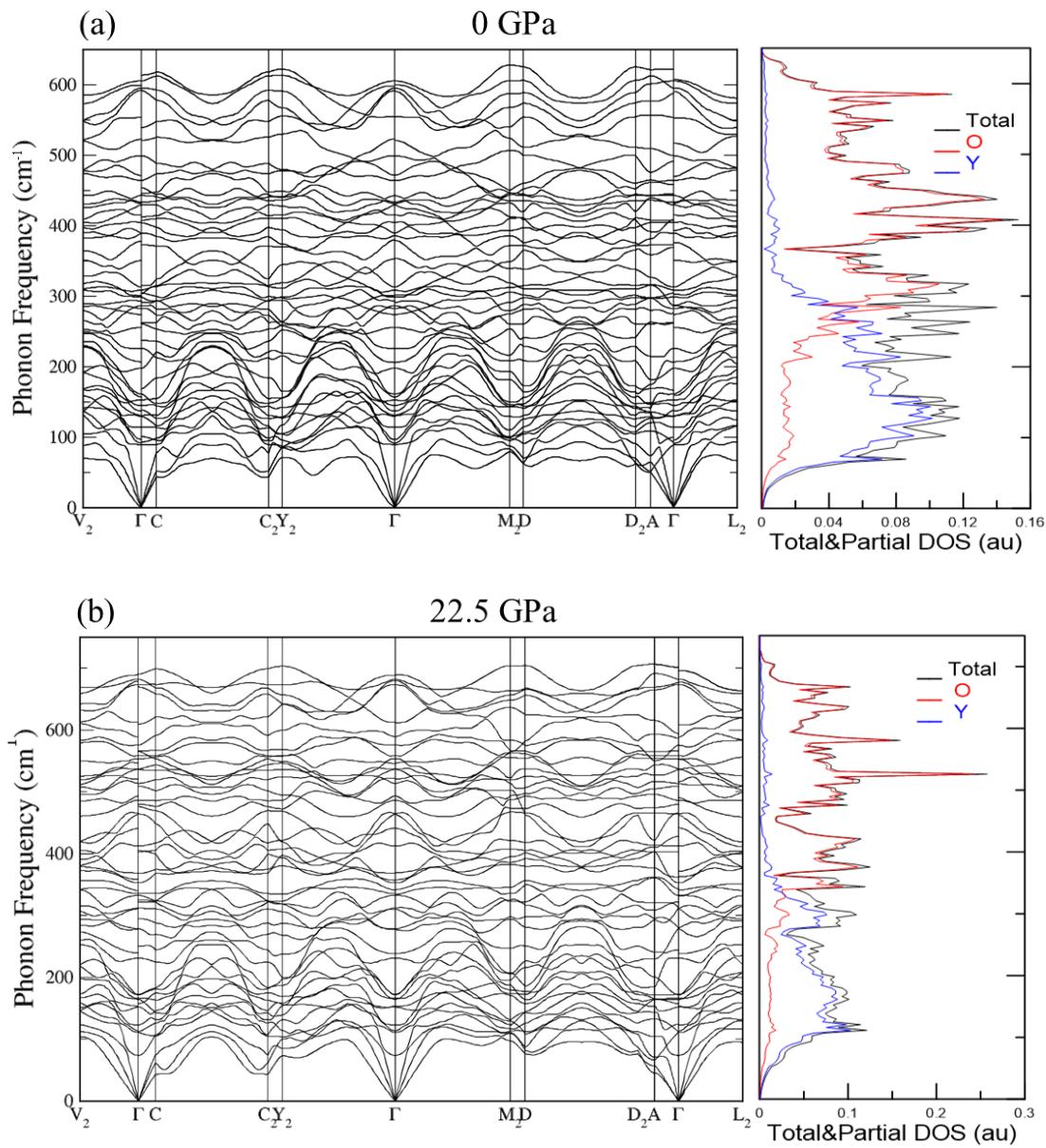


Figure S10. Phonon dispersion curves and respective total and partial density of states (DOS) of monoclinic Y_2O_3 at (a) 0 GPa and (b) 22.5 GPa.

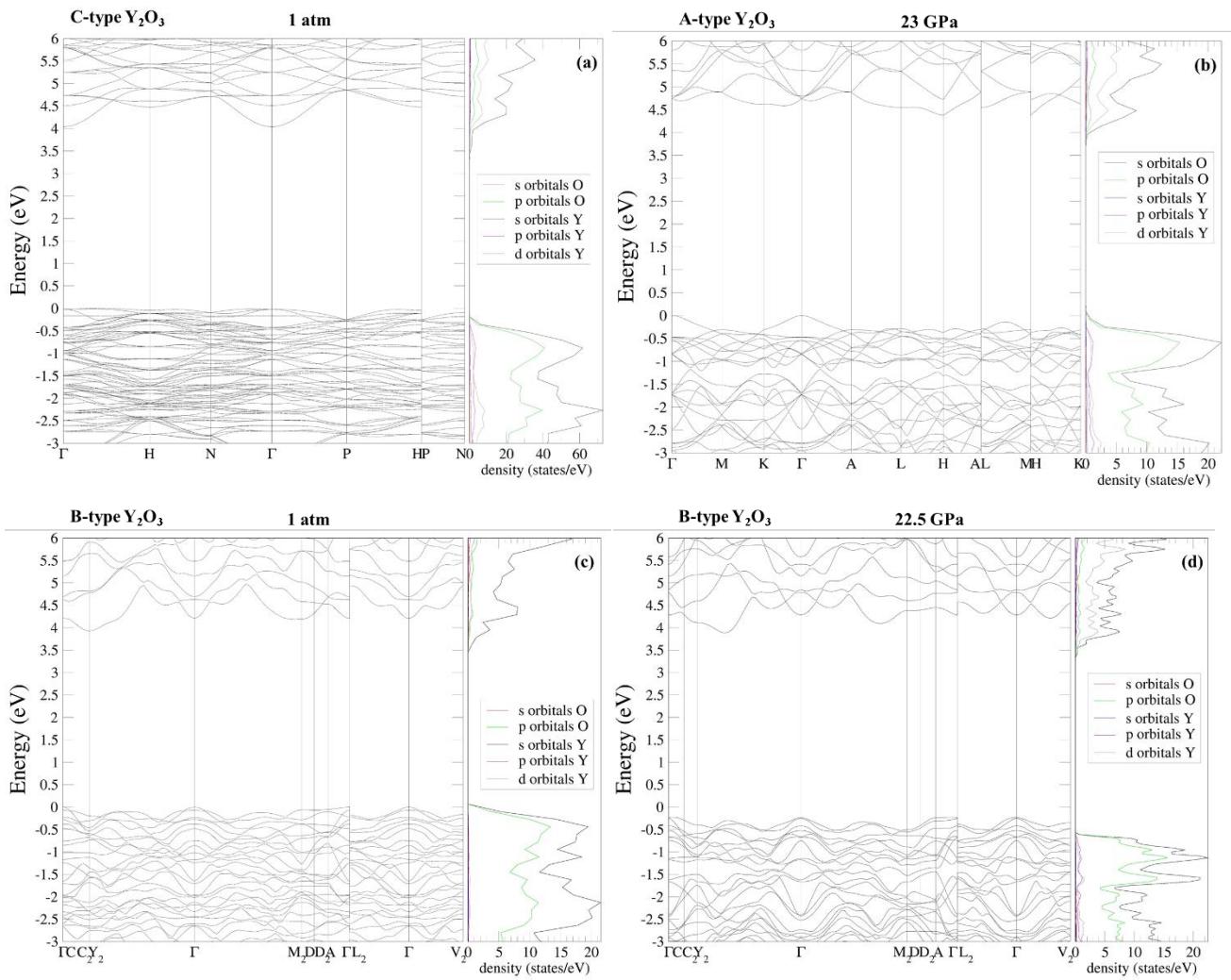


Figure S11. Band structure curves and respective total and partial density of states (DOS) of (a) C-type (1 atm), (b) A-type (23.0 GPa), and B type at (c) 1 atm and (d) 22.5 GPa.

References:

- [S1] Li Z, Wang J, Wang L, Bai X, Song H, Zhou Q, et al. The pressure induced amorphization and behavior of octahedron in Y₂O₃/Eu³⁺ nanotubes. Mater Res Express 2014;1:025013. <https://doi.org/10.1088/2053-1591/1/2/025013>.
- [S2] Zhang Q, Wu X, Qin S. Pressure-induced phase transition of B-type Y₂O₃. Chinese Phys B 2017;26:090703. <https://doi.org/10.1088/1674-1056/26/9/090703>.