

β -Bi₂O₃ under compression: Optical and elastic properties and electron density topology analysis

A. L. J. Pereira,^{a,b} O. Gomis,^c* J. A. Sans,^a J. Contreras-García,^d F.J. Manjón,^a P. Rodríguez-Hernández,^e A. Muñoz,^e and A. Beltrán^f

^a Instituto de Diseño para la Fabricación y Producción Automatizada, MALTA Consolider Team, Universitat Politècnica de València, València, Spain

^b Departamento de Física, Divisão de Ciências Fundamentais, Instituto Tecnológico de Aeronáutica, São José dos Campos, Brazil

^c Centro de Tecnologías Físicas: Acústica, Materiales y Astrofísica, MALTA Consolider Team, Universitat Politècnica de València, València, Spain

^d Laboratoire de Chimie Théorique, Université Pierre et Marie Curie, F-75005 Paris, France

^e Departamento de Física, Instituto de Materiales y Nanotecnología, MALTA Consolider Team, Universidad de La Laguna, La Laguna, Tenerife, Spain

^f Departament de Química Física i Analítica, MALTA Consolider Team, Universitat Jaume I, Castello de la Plana (Spain)

Supplemental Material

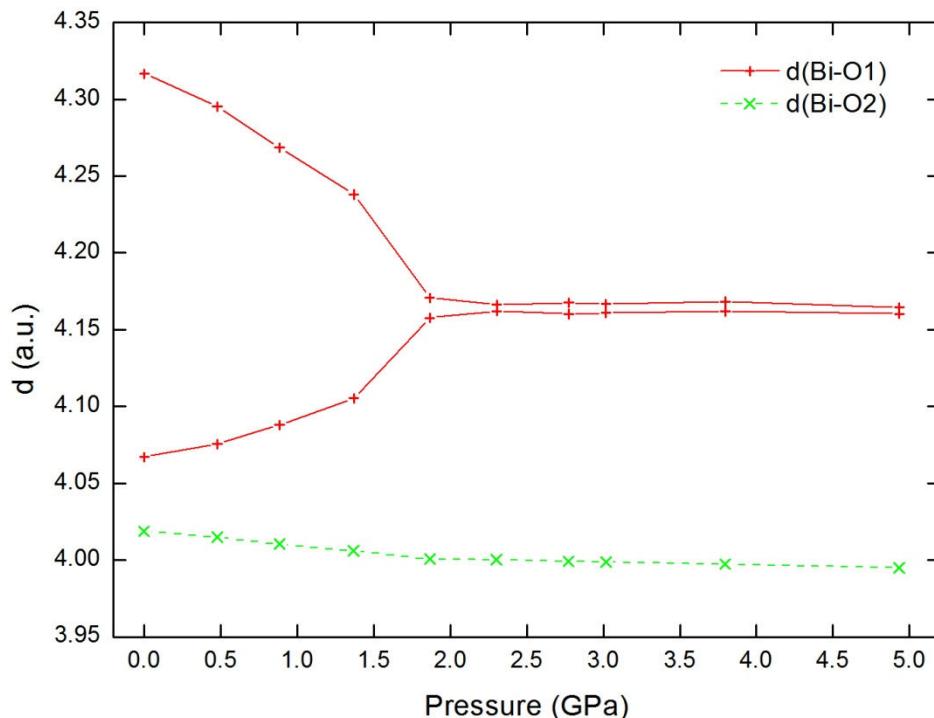


Figure S1. (Color online) Evolution of Bi-O distances upon compression of Bi₂O₃. Equalization of first and second neighbor distances for Bi-O1 is observed at around 2 GPa.

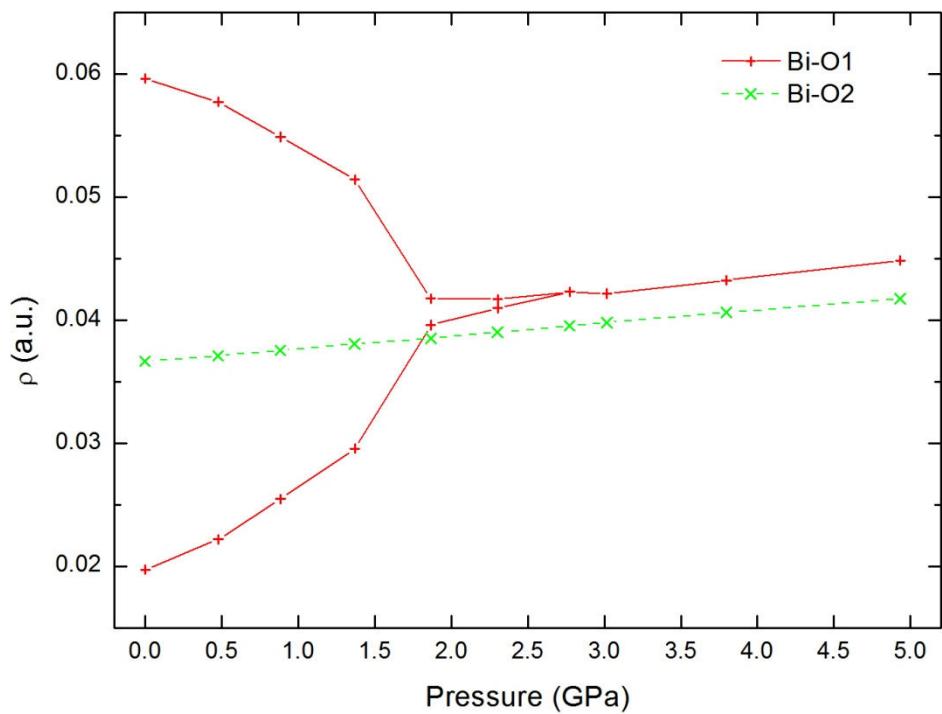


Figure S2. (Color online) Evolution of the electron density at the bcp along the Bi and O line upon compression of Bi_2O_3 .

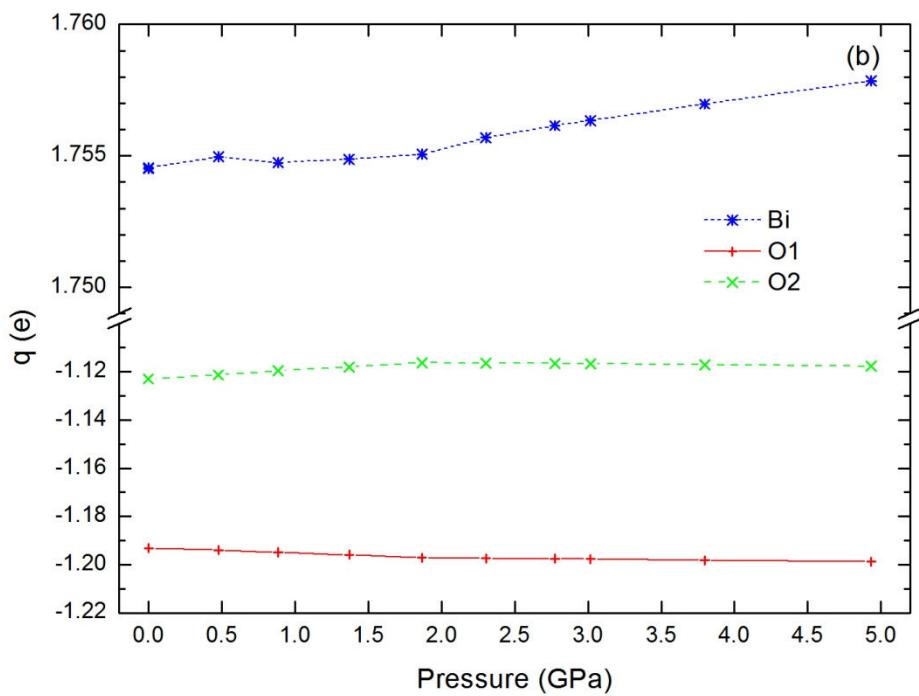
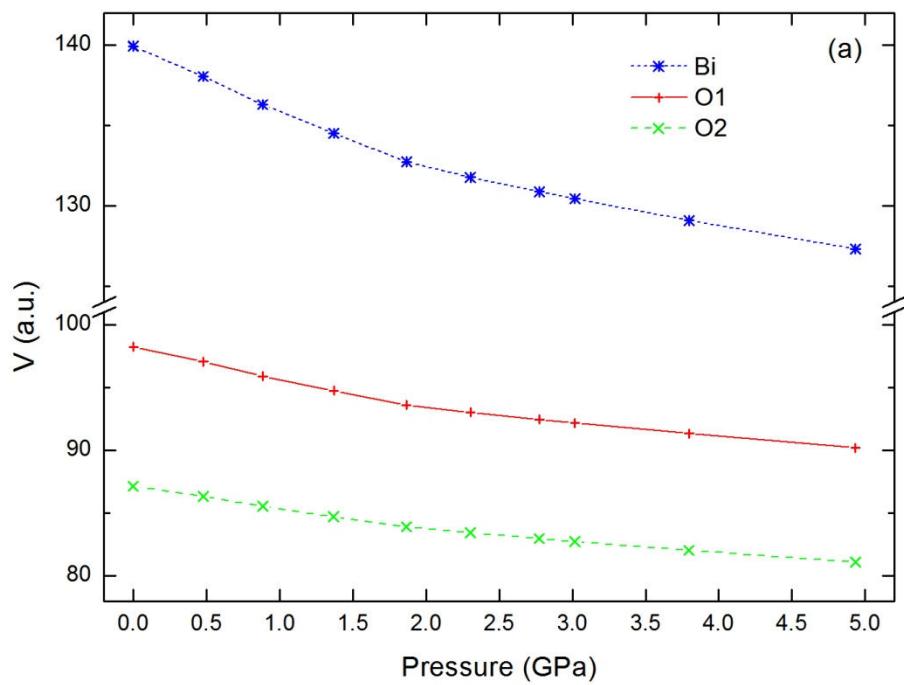


Figure S3. (Color online) Evolution of Bader atomic basins for Bi_2O_3 upon compression: volumes (a), charges (b).

Table S1. List of critical points (CPs) for the β and β' phases. bcp stands for bond critical point, rcp for ring critical point, and ccp for cage critical point. The topological class is summarized in the column TOTAL, where the number of each type of critical points is collected after taking into account their multiplicity. The number of critical points was in all cases coherent, providing a Morse sum equals to zero in both cases (20-48+40-12).

PHASE β					PHASE β'				
N	CP	Symmetry	multiplicity	TOTAL	N	CP	Symmetry	multiplicity	TOTAL
1	O1	C1	8	20	1	O1	C2	8	20
2	O2	C1	4		2	O2	C2v	4	
3	Bi	C1	8		3	Bi	Cs	8	
4	bcp	C1	8	48	4	bcp	Cs	8	48
5	bcp	C1	8		5	bcp	C1	16	
6	bcp	C1	8		6	bcp	C1	16	
7	bcp	C1	8		7	bcp	Cs	8	
8	bcp	C1	8						
9	bcp	C1	8						
10	rcp	C1	8	40	8	rcp	Cs	8	40
11	rcp	C1	8		9	rcp	Cs	8	
12	rcp	C1	8		10	rcp	I	8	
13	rcp	C1	8		11	rcp	C1	16	
14	rcp	C1	8						
15	ccp	C1	8	12	12	ccp	Cs	8	12
16	ccp	S2	2		13	ccp	D2d	2	
17	ccp	S2	2		14	ccp	D2d	2	