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

Vibrational Properties of Metastable Orthorhombic Bi_2Se_3

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SUPPLEMENTARY MATERIAL

The table S1 presents the atomic positions of the Bi2Se3 in the unitary cells used for the calculations.

Table S1: Unitary cell for Bi2Se3 Phases

Pnma				R-3m			
Atom	X	y	z	Atom	x	y	z
Bi	0.5007	0.2500	0.1721	Bi	0	0	0
Bi	0.4993	0.7500	0.8279	Bi	0	0	0.5990
Bi	0.9993	0.7500	0.6721	Bi	0.6667	0.3333	0.7443
Bi	0.0007	0.2500	0.3279	Bi	0.6667	0.3333	0.9323
Bi	0.6641	0.7500	0.4631	Bi	0.3333	0.6667	0.0677
Bi	0.3359	0.2500	0.5369	Bi	0.3333	0.6667	0.2567
Bi	0.8358	0.2500	0.9631	Bi	0	0	0.4010
Bi	0.1641	0.7500	0.0369	Se	0	0	0.5990
Se	0.6265	0.7500	0.0557	Se	0.6667	0.3333	0.3333
Se	0.3734	0.2500	0.9442	Se	0.6667	0.3333	0.5433
Se	0.8734	0.2500	0.5558	Se	0.3333	0.6667	0.6667
Se	0.1266	0.7500	0.4442	Se	0.3333	0.6667	0.8766
Se	0.7213	0.2500	0.2981	Se	0	0	0.7900
Se	0.2786	0.7500	0.7019	Se	0.6667	0.3333	0.1234
Se	0.7786	0.7500	0.7981	Se	0.3333	0.6667	0.8766
Se	0.2213	0.2500	0.2019	Se	0.3333	0.6667	0.4567
Se	0.4445	0.7500	0.3672				
Se	0.5554	0.2500	0.6328				
Se	0.0554	0.2500	0.8672				
Se	0.9445	0.7500	0.1328				

In the table below are presented all Raman Modes obtained in the DFT calculation for the both phases, the R-3m and the Pnma. The lines highlighted in yellow are the most active modes.

Table S2: Raman Modes, Symmetry and Activities from DFT calculation.

Rhombohedral Phase (R-3M)					Orthorhombic Phase (Pnma)			
Mode	Symmetry	Frequency(cm^{-1})	Activity		Mode	Symmetry	Frequency(cm^{-1})	Activity
5	A_{1g}	180.8445	146115		1	B_{1u}	182.943	0.0590
6	A_{2u}	170.0389	0.0055		2	B_{3u}	178.6646	0.0003
9	A_{2u}	145.3084	0.4724		3	B_{2g}	174.6488	2963.1
10	E_g	141.7409	75965		4	A_g	172.938	11166.

16	E_u	134.5128	3.9732
26	E_u	88.9838	4.0431
28	A_{1g}	76.79783	19341.
31	E_g	43.91538	195.63

5	B_{3u}	170.2593	0.0084
6	B_{2g}	168.9988	4194.0
7	B_{1u}	164.6217	0.0010
8	A_g	163.1819	3564.3
9	B_{1u}	158.639	0.0032
10	A_g	156.6652	116478
11	B_{2g}	155.2874	3254.8
12	B_{3u}	149.8731	0.0367
13	B_{2g}	144.3683	5260.0
14	B_{3g}	137.3832	291.59
15	B_{1g}	135.6143	2137.4
16	B_{1u}	134.0706	3.5523
17	B_{3u}	132.861	0.0006
18	B_{2g}	132.2939	185.61
19	B_{2u}	131.5038	0.0208
20	A_g	130.7787	8137.8
21	A_u	129.6016	0.0091
22	B_{1g}	128.7876	128.19
23	B_{2u}	128.309	3.3394
24	A_g	127.0941	4973.6
25	A_u	126.3647	0.0058
26	B_{3g}	125.6311	11741.
27	B_{1u}	123.2143	0.0968
28	B_{2g}	122.9879	79.298
29	A_g	121.7258	10486.
30	B_{3u}	121.4234	0.0040
31	B_{3g}	113.6492	404.07
32	B_{1g}	109.1341	104.93
33	B_{3u}	99.51381	2.9858
34	A_u	95.43844	0.0004
35	A_g	88.33544	1455.7
36	B_{2u}	87.67187	0.0294
37	B_{1u}	86.33217	0.0003
38	B_{2g}	86.04035	724.48
39	B_{1u}	74.07029	0.0322
40	B_{2g}	72.50459	1082.6
41	B_{3u}	71.65241	0.0005
42	B_{2g}	69.39349	228.13
43	A_g	58.85512	469.01
44	B_{1u}	58.64523	0.0078
45	B_{3u}	53.84063	0.0008
46	B_{3g}	50.91584	1034.5
47	B_{1g}	50.71975	175.21
48	B_{2u}	48.75048	2.1070
49	A_u	45.30886	0.0002
50	A_g	43.39543	2366.1
51	B_{1u}	39.76913	0.1143
52	B_{3g}	39.30506	1498.5
53	A_g	35.4169	521.36
54	B_{1g}	35.37753	0.9160
55	B_{2g}	32.79967	314.12
56	B_{3u}	24.58311	0.0259
57	A_u	21.15165	0.0010

INCAR (VASP FILE) used in the SCF Pnma Bi2Se3 calculations.

SYSTEM = Bi2Se3

NWRITE = 3

LPLANE = .TRUE.

LSCALU = .FALSE.

NSIM = 1

NCORE = 4

ISTART = 1

ICHARG = 1

ALGO = VeryFast

PREC = Accurate

LREAL = AUTO

IBRION = 2

ISIF = 3

NSW = 200

EDIFFG = -0.01

ISMEAR = 1

SIGMA = 0.1

NWRITE = 3

LREAL = .FALSE.

IALGO = 38

ADDGRID = .TRUE.

INCAR (VASP FILE) used in the SCF R-3m Bi2Se3 calculations.

SYSTEM = Bi2Se3

NWRITE = 3

LPLANE = .TRUE.

LSCALU = .FALSE.

NSIM = 1

NCORE = 4

ISTART = 1

ICHARG = 1

ALGO = VeryFast

PREC = Accurate

LREAL = AUTO

IBRION = 2

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ADDGRID = .TRUE.