

Phonons in cubic bulk PbTiO_3 with SIESTA

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(Dated: June 1, 2010)

PACS numbers: 73.30.+y, 73.40.Rw, 73.40.Qv, 73.90.+f

I. PHONONS IN CUBIC BULK PbTiO_3 AT THE BORDER OF THE FIRST BRILLOUIN ZONE

- Monkhorst-Pack grid: $6 \times 6 \times 6$.
- Mesh cutoff: 1200 Ry
- Force constant matrix computed in a $2 \times 2 \times 2$ supercell in real space (40 atoms in the supercell).
- All the atoms in the supercell in real space displaced along the three cartesian directions ± 0.03 bohrs.
- Force constant matrix computed at the corresponding theoretical lattice constant:
 - LDA lattice constant = 7.36051 bohr = 3.895012 Å.
 - GGA-Wu Cohen lattice constant = 7.40679 bohr = 3.919505 Å.

TABLE I. Phonons at Γ . LO-TO splitting not considered. Frequencies in cm^{-1} . 1200 Ry of Mesh Cutoff. Displacement: 0.03 bohr

Eigenvalue number	Degeneration	LDA (Ceperley-Alder)	GGA (Wu-Cohen)
1	triple	-112	-138
2	triple	0	0
3	triple	145	120
4	triple	220	238
5	triple	519	490

TABLE II. Phonons at X. Frequencies in cm^{-1} . 1200 Ry of Mesh Cutoff. Displacement: 0.03 bohr.

Eigenvalue number	Degeneration	LDA (Ceperley-Alder)	GGA (Wu-Cohen)
1	doble	45	48
2	single	110	112
3	doble	140	90
4	doble	170	171
5	single	266	274
6	doble	280	285
7	single	289	276
8	doble	495	465
9	single	508	501
10	single	740	714

TABLE IV. Phonons at R. Frequencies in cm^{-1} . 1200 Ry of Mesh Cutoff. Displacement: 0.03 bohr

Eigenvalue number	Degeneration	LDA (Ceperley-Alder)	GGA (Wu-Cohen)
1	triple	-84	-60
2	triple	61	66
3	triple	371	374
4	triple	425	408
5	doble	496	461
6	single	833	811

TABLE III. Phonons at M. Frequencies in cm^{-1} . Eigenfrequencies ordered according to the LDA results. 1200 Ry of Mesh Cutoff. Displacement: 0.03 bohr

Eigenvalue number	Degeneration	LDA (Ceperley-Alder)	GGA (Wu-Cohen)
1	single	-50	9
2	doble	42	43
3	single	55	55
4	single	150	105
5	doble	233	237
6	doble	302	306
7	single	436	419
8	doble	438	424
9	single	458	437
10	single	526	491
11	single	800	778