

STISHOVITE. PBE FUNCTIONAL. FHI-TM (HAM) TYPE PSEUDOPOTENTIALS.

Ac_{cell}=B_{cell}=8.0040144448 a.u., C_{cell}=5.0756950752 a.u.

Si: (0 0 0)

O: (0.307071; 0.307071; 0)

E_{CUT} – test (NGKPT = 4x4x4)

	E _{TOTAL} , eV	Pressure, GPa
E _{cut} = 10 Ha	-1870.09821581027	-272.68
E _{cut} = 20 Ha	-1949.71870137093	-138.61
E _{cut} = 30 Ha	-1962.76033450275	-17.524
E _{cut} = 35 Ha	-1963.39748094866	-3.1252
E_{cut} = 40 Ha	-1963.47186413440	-0.22660
E _{cut} = 45 Ha	-1963.48267789760	-0.29418
E _{cut} = 50 Ha	-1963.50418395192	-0.56239
E _{cut} = 60 Ha	-1963.54547847813	-0.35940

NGKPT-test (E_{CUT} = 40 Ha).

	E _{TOTAL} , eV	Pressure, GPa
2x2x2	-1964.15861439541	-1.3703
2x2x4	-1963.48009594758	-0.23826
4x4x4	-1963.47186413580	-0.22677
4x4x6	-1963.45799459735	-0.20567
6x6x6	-1963.45796846296	-0.21847
6x6x8	-1963.45756825860	-0.21822
8x8x8	-1963.45756179290	-0.20610

Gamma-test.

	4x4x6, 40 Ha	8x8x8, 40 Ha	4x4x6, 60 Ha	4x4x6, 80 Ha
E _{TOTAL} , eV	-1963.45799	-1963.45756	-1963.53164	-1963.54916
Pressure, GPa	-0.2181	-0.2188	-0.3690	-0.0524
F-sum rule	0.99995 0.99942	0.99999 0.99995	0.99994 0.99942	0.99995 0.99943
Z(Si) – Born charge tensor components	3.83711 0.40913 4.08234	3.83702 0.40907 4.08156	3.83711 0.40896 4.08231	3.83708 0.40891 4.08232
Z(O) – Born charge tensor components	-1.91882 -0.59367 -2.03731	-1.91910 -0.59389 -2.04112	-1.91778 -0.59297 -2.03685	-1.91756 -0.59319 -2.03714
ε _{∞ 11}	3.3944	3.3961	3.3935	3.3933
ε _{∞ 33}	3.5545	3.5627	3.5538	3.5535

ω , cm ⁻¹	-58.9	-58.9	-33.8	47.5
<100>	-44.9	-44.9	35.8	47.8
	-44.8	-44.8	35.9	51.9
	224.6	224.6	230.6	239.8
	367.8	367.8	368.8	370.4
	423.3	423.3	425.3	427.0
	528.7	528.7	531.8	533.3
	530.6	530.5	533.7	534.8
	550.4	550.3	554.2	560.6
	550.4	550.3	554.2	560.6
	575.9	575.9	578.6	582.0
	623.5	623.5	624.7	627.5
	673.6	673.6	674.1	675.0
	711.3	711.2	717.5	717.1
	718.5	718.5	720.9	724.9
	794.6	794.6	796.8	796.9
	900.0	900.0	905.0	904.5
	990.5	990.4	992.8	992.7

Setting ixc=1 (LDA), I get:

	4x4x6, 40 Ha
E _{TOTAL} , eV	-1957.25141
Pressure, GPa	-4.569
F-sum rule	0.99933
Z(Si) – Born charge tensor components	3.82652 0.39959 4.07945
Z(O) – Born charge tensor components	-1.91276 -0.59082 -2.03429
$\epsilon_{\infty 11}$	3.46744
$\epsilon_{\infty 33}$	3.61450
ω , cm ⁻¹ <100>	3.2 3.2 16.0 213.3 368.2 429.0 522.2 532.5 553.6 563.5 563.5 646.2 668.6 723.7 733.7 800.8 900.5 997.4

