

MgO. LDA (ixc=7). TM-pseudopotentials. (acell=7.960 a.u.)

E_{CUT} – test (NGKPT = 4x4x4)

	E _{TOTAL} , eV	Pressure, GPa
Ecut = 10 Ha	-460.71171	-207.30
Ecut = 20 Ha	-482.29693	-78.96
Ecut = 30 Ha	-484.98784	-3.892
Ecut = 40 Ha	-485.08526	3.406
Ecut = 50 Ha	-485.09518	3.100
Ecut = 60 Ha	-485.10343	3.311
Ecut = 70 Ha	-485.10538	3.425
Ecut = 80 Ha	-485.10575	3.439
Ecut = 90 Ha	-485.10595	3.440
Ecut = 100 Ha	-485.10610	3.443

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

	E _{TOTAL} , eV	Pressure, GPa
2x2x2	-485.07775	3.437
4x4x4	-485.08526	3.407
6x6x6	-485.08524	3.404
8x8x8	-485.08524	3.406
10x10x10	-485.08524	3.405
12x12x12	-485.08524	3.404

Phonons at the Gamma-point.

	4x4x4, 40 Ha	4x4x4, 60 Ha	8x8x8, 40 Ha	12x12x12, 60 Ha
E _{TOTAL} , eV	-485.08526	-485.10343	-485.08524	-485.10339
Pressure, GPa	3.4079	3.3117	3.4058	3.3102
F-sum rule	1.00432	1.00427	1.00005	0.999984
Z(Mg)	1.93822	1.93827	1.94445	1.94455
Z(O)	-2.04125	-2.04091	-1.94527	-1.94442
ε _∞	3.18459	3.18369	3.12672	3.12494
ω, cm ⁻¹	104.37	104.42	6.20	0.72
	104.37	104.42	6.20	0.72
	107.36	107.43	6.20	0.72
	461.26	461.16	440.84	440.64
	461.26	461.16	440.84	440.64
	732.29	732.25	724.19	724.17