SACADA Database Code: 505

Topology: 4^3T141

# of independent nodes (IN): 3
Transitivity: [3663]
Space Group: Fmmm
Pearson: oF48
Coordination Number (CN): 4

Year: 2017

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^3T141 (SACADA #505)		3.246		0.749	383.8	413.3	76.6	SACADA[1]
G218								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

10609.8971	43.8110	1508.9578	0.0000	0.0000	0.0000
43.8110	9329.5399	1300.8043	-0.0000	0.0000	-0.0000
1508.9578	1300.8043	8955.4360	-0.0000	0.0000	-0.0000
0.0000	-0.0000	0.0000	3760.6494	-0.0000	0.0000
0.0000	0.0000	0.0000	-0.0000	4186.5791	-0.0000
0.0000	-0.0000	-0.0000	0.0000	-0.0000	4157.5573

[1] We apply the density functional theory (DFT) approach by using the Vienna Ab Initio Simulation Package (VASP) to calculate the total energy and properties of carbon allotropes.

DFT calculations

We apply the density functional theory (DFT) approach by using the Vienna Ab Initio Simulation Package (VASP) package [6] to calculate the total energy of carbon allotropes. The Generalized Gradient Approximation [7] (GGA) for exchange-correlational functional is used everywhere. The energy cutoff set to 600 eV. Fully automatic Γ-centered k-points mesh with a reciprocal-space resolution of $2\pi \times 0.025$ Å^{-1} is applied. We used tetrahedron method with Blöchl corrections to perform the k-point integration. The convergence thresholds are set at 10^{-6} eV for energy and 10^{-5} eV Å^{-1} for ionic forces. Polycrystalline elastic moduli — the bulk modulus, the shear modulus, Young's modulus, and the Poisson's ratio ν — have been calculated within the Voigt–Reuss–Hill [8] approximation. The Vicker's hardness H_v has been estimated according to Oganov's model [9].