SACADA Database Code: 378

Topology: 4^3T173

# of independent nodes (IN): 3
Transitivity: [3883]
Space Group: Ima2
Pearson: oI24
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
4^3T173 (SACADA #378)		3.234		0.875	375.2	381.2	69.0	SACADA[1]
G58								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

9929.7040	549.3555	630.1286	-0.0000	0.0000	0.0000
549.3555	8991.8924	943.4796	-0.0000	0.0000	0.0000
630.1286	943.4796	10697.2747	0.0000	-0.0000	0.0000
-0.0000	0.0000	0.0000	3440.5281	-0.0000	0.0000
0.0000	0.0000	-0.0000	-0.0000	3140.0636	-0.0000
0.0000	0.0000	0.0000	0.0000	-0.0000	3563.3477

[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].