SACADA Database Code: 438

Topology: 4^3T3

# of independent nodes (IN): 3
Transitivity: [3343]
Space Group: Cmmm
Pearson: oS10
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
4^3T3 (SACADA #438)		3.369		1.523	-	-	-	SACADA[1]
G138								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

9747.9562	848.9209	187.8660	0.0000	0.0000	0.0000
848.9209	9517.9311	1171.6981	0.0000	0.0000	0.0000
187.8660	1171.6981	9823.4646	-0.0000	0.0000	-0.0000
0.0000	0.0000	-0.0000	-2581.0709	-0.0000	0.0000
0.0000	0.0000	0.0000	-0.0000	2318.6254	0.0000
0.0000	0.0000	-0.0000	0.0000	0.0000	2635.9174

[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].