SACADA Database Code: 407

Topology: 4^3T175

# of independent nodes (IN): 3
Transitivity: [3675]
Space Group: Cmmm
Pearson: oS20
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
4^3T175 (SACADA #407)		3.290		0.920	366.1	373.6	67.8	SACADA[1]
G100								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

10947.7932	1130.2861	19.2770	0.0000	-0.0000	0.0000
1130.2861	8900.3007	166.9715	0.0000	-0.0000	0.0000
19.2770	166.9715	10575.2770	-0.0000	0.0000	-0.0000
0.0000	0.0000	-0.0000	4675.4126	0.0000	0.0000
-0.0000	-0.0000	-0.0000	0.0000	1875.1021	0.0000
0.0000	0.0000	-0.0000	0.0000	0.0000	3706.2117

[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].