SACADA Database Code: 371

Topology: 4^5T50

# of independent nodes (IN): 5
Transitivity: [5(12)72]
Space Group: P-1
Pearson: aP10
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
4^5T50 (SACADA #371)		3.260		0.990	373.0	374.1	67.3	SACADA[1]
G35								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

8570.1963	1335.5139	914.1962	327.0830	199.8969	16.8386
1335.5139	8531.9292	1289.6847	492.7908	155.1040	141.3237
914.1962	1289.6847	9410.3609	16.2769	-297.7257	-14.4539
327.0830	492.7908	16.2769	3695.5367	-247.2421	6.6613
199.8969	155.1040	-297.7257	-247.2421	4082.7750	172.0651
16.8386	141.3237	-14.4539	6.6613	172.0651	3346.2782

[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].