SACADA Database Code: 433

Topology: 4^9T9

# of independent nodes (IN): 9
Transitivity: [9(16)(11)4]
Space Group: I2
Pearson: mS32
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
4^9T9 (SACADA #433)		3.375		1.043	382.5	403.1	74.1	SACADA[1]
G133								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

8846.9122	925.5202	1551.6397	0.0000	0.0000	-104.7419
925.5202	10194.2401	992.8702	0.0000	-0.0000	-80.4122
1551.6397	992.8702	8476.7286	0.0000	-0.0000	350.4879
0.0000	0.0000	0.0000	4046.4043	266.5591	-0.0000
0.0000	-0.0000	-0.0000	266.5591	4134.9312	-0.0000
-104.7419	-80.4122	350.4879	-0.0000	-0.0000	4017.5191

[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].