SACADA Database Code: 518

Topology: 4^3T190

# of independent nodes (IN): 3
Transitivity: [3663]
Space Group: Pmma
Pearson: oP10
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
4^3T190 (SACADA #518)		3.357		0.802	393.5	412.6	75.7	SACADA[1]
G237								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

10756.7973	517.6084	737.8024	0.0000	-0.0000	-0.0000
517.6084	9583.2773	2196.3421	0.0000	-0.0000	0.0000
737.8024	2196.3421	8228.5554	-0.0000	-0.0000	-0.0000
0.0000	0.0000	-0.0000	4014.6100	0.0000	0.0000
-0.0000	-0.0000	0.0000	0.0000	3887.7453	0.0000
-0.0000	0.0000	-0.0000	0.0000	0.0000	4577.9926

[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].