SACADA Database Code: 444

Topology: 4^6T36

# of independent nodes (IN): 6
Transitivity: [6(12)71]
Space Group: P21
Pearson: mP12
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
4^6T36 (SACADA #444)		3.320		1.160	368.0	382.8	70.0	SACADA[1]
G150								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

8805.3642	889.8421	1101.4118	0.0000	-0.0000	-318.8340
889.8421	8493.1290	1408.3293	-0.0000	-0.0000	162.3930
1101.4118	1408.3293	9052.1982	-0.0000	-0.0000	-300.9576
0.0000	-0.0000	-0.0000	3567.0082	-542.7176	-0.0000
-0.0000	-0.0000	-0.0000	-542.7176	4049.9024	0.0000
-318.8340	162.3930	-300.9576	-0.0000	0.0000	3894.5719

[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].