SACADA Database Code: 420

Topology: 4^4T85

# of independent nodes (IN): 4
Transitivity: [4951]
Space Group: P21/c
Pearson: mP16
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
4^4T85 (SACADA #420)		3.408		0.767	403.4	456.7	85.8	SACADA[1]
G120								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

8624.4633	1488.6138	1369.6182	0.0000	-0.0000	-85.9337
1488.6138	9798.7762	742.7140	-0.0000	-0.0000	351.8621
1369.6182	742.7140	10733.6013	0.0000	-0.0000	-250.3149
0.0000	-0.0000	0.0000	4862.3653	291.9470	0.0000
-0.0000	-0.0000	-0.0000	291.9470	4426.8798	-0.0000
-85.9337	351.8621	-250.3149	0.0000	-0.0000	5180.9158

[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].