SACADA Database Code: 417

Topology: 4^4T117

# of independent nodes (IN): 4
Transitivity: [4(10)51]
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
4^4T117 (SACADA #417)		3.503		0.894	399.0	474.4	89.9	SACADA[1]
G117								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

10728.3187	267.4612	1172.5934	0.0000	-0.0000	246.7680
267.4612	10949.7435	652.7534	0.0000	-0.0000	-395.4762
1172.5934	652.7534	10046.8869	-0.0000	-0.0000	96.2284
0.0000	0.0000	-0.0000	4674.0301	-385.6278	0.0000
-0.0000	-0.0000	-0.0000	-385.6278	4761.8524	0.0000
246.7680	-395.4762	96.2284	0.0000	0.0000	4450.0651

[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].