SACADA Database Code: 384

Topology: 4^7T24

# of independent nodes (IN): 7
Transitivity: [7(15)(15)7]
Space Group: C2
Pearson: mS28
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
4^7T24 (SACADA #384)		3.504		0.893	402.5	467.5	88.3	SACADA[1]
G68								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

10109.8608	510.0581	1176.4006	0.0000	-0.0000	-451.8362
510.0581	11504.1299	684.2837	-0.0000	-0.0000	-89.9357
1176.4006	684.2837	9895.4221	0.0000	-0.0000	574.0298
0.0000	-0.0000	0.0000	4379.6696	-132.8734	0.0000
-0.0000	-0.0000	-0.0000	-132.8734	4881.5765	-0.0000
-451.8362	-89.9357	574.0298	0.0000	0.0000	4464.5848

[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].