SACADA Database Code: 66

Topology: 4/5/t1

# of independent nodes (IN): 1
Transitivity: [1322]
Space Group: I41/a
Pearson: tI16
Coordination Number (CN): 4

Year: 2015

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4/5/t1 (SACADA #66)		3.575		0.837	375.8	486.1	93.0	SACADA[1]
I41/a					346			doi: 10.1103/PhysRevB.91.214104
BT8		3.508			333			doi: 10.1103/PhysRevB.94.174102

Elasticity tensor (kBar)[1]

10663.2199	420.1187	886.8770	23.5912	0.0000	0.0000
420.1187	10663.2199	886.8770	-23.5912	0.0000	0.0000
886.8770	886.8770	8257.6695	-0.0000	0.0000	-0.0000
23.5912	-23.5912	-0.0000	5178.4688	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	5070.2921	-0.0000
-0.0000	-0.0000	0.0000	0.0000	-0.0000	5070.2921

[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].

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