SACADA Database Code: 413

Topology: 4^3T176

# of independent nodes (IN): 3
Transitivity: [3442]
Space Group: Fmmm
Pearson: oF28
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
4^3T176 (SACADA #413)		3.317		1.387	-	-	-	SACADA[1]
G110								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

10083.4038	1307.8000	601.6355	0.0000	0.0000	0.0000
1307.8000	7700.4922	1702.5654	-0.0000	-0.0000	0.0000
601.6355	1702.5654	8306.8617	-0.0000	0.0000	0.0000
0.0000	-0.0000	-0.0000	2893.4931	-0.0000	0.0000
0.0000	-0.0000	0.0000	-0.0000	-736.7609	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	2725.1515

[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].