SACADA Database Code: 479

Topology: 4^3T182

# of independent nodes (IN): 3
Transitivity: [3772]
Space Group: C2/c
Pearson: mS24
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
4^3T182 (SACADA #479)		3.195		0.937	367.0	367.7	66.1	SACADA[1]
G187								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

7146.2094	1827.9487	1142.9611	0.0000	-0.0000	-224.9890
1827.9487	9190.0325	1019.7460	-0.0000	-0.0000	812.3217
1142.9611	1019.7460	8858.5666	-0.0000	-0.0000	-381.1425
0.0000	-0.0000	-0.0000	3068.7122	237.8745	0.0000
0.0000	-0.0000	-0.0000	237.8745	4423.6923	0.0000
-224.9890	812.3217	-381.1425	0.0000	0.0000	4062.8816

[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].