SACADA Database Code: 441

Topology: 4^3T179

# of independent nodes (IN): 3
Transitivity: [3753]
Space Group: C2/m
Pearson: mS16
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
4^3T179 (SACADA #441)		3.151		0.936	363.5	336.1	57.0	SACADA[1]
G146								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

9615.6276	877.6139	1043.9555	-0.0000	-0.0000	-36.7656
877.6139	8533.6903	1340.5217	-0.0000	0.0000	-163.4076
1043.9555	1340.5217	8070.8135	-0.0000	0.0000	-471.2015
0.0000	-0.0000	-0.0000	3376.2304	-112.4290	-0.0000
-0.0000	0.0000	0.0000	-112.4290	2244.8869	0.0000
-36.7656	-163.4076	-471.2015	-0.0000	0.0000	3930.7834

[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].