SACADA Database Code: 440

Topology: 4^3T178

# of independent nodes (IN): 3
Transitivity: [3774]
Space Group: Cmm2
Pearson: oS16
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
4^3T178 (SACADA #440)		3.013		1.077	355.0	295.3	44.1	SACADA[1]
G145								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

9015.1558	853.2829	1070.0963	1.8360	0.0233	-1.2547
853.2829	8324.1276	1195.7701	2.8647	0.9842	0.5161
1070.0963	1195.7701	8387.6055	11.9154	-2.0829	1.4766
1.8360	2.8647	11.9154	3364.9994	2.7274	-3.2689
0.0233	0.9842	-2.0829	2.7274	2911.0660	2.1002
-1.2547	0.5161	1.4766	-3.2689	2.1002	1653.5396

[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].