SACADA Database Code: 193

Topology: 4^3T139

# of independent nodes (IN): 3
Transitivity: [3895]
Space Group: Pm-3m
Pearson: cP96
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
4^3T139 (SACADA #193)		2.651		1.313	265.5	231.6	36.9	SACADA[1]
		2.7	1.85		279	219		doi: 10.1039/c5ta01045d

Elasticity tensor (kBar)[1]

6210.2256	877.1421	877.1421	-0.0000	0.0000	0.0000
877.1421	6210.2256	877.1421	0.0000	-0.0000	0.0000
877.1421	877.1421	6210.2256	-0.0000	-0.0000	-0.0000
-0.0000	0.0000	-0.0000	2108.5261	0.0000	-0.0000
0.0000	-0.0000	-0.0000	0.0000	2108.5261	0.0000
0.0000	0.0000	0.0000	-0.0000	0.0000	2108.5261

[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].