SACADA Database Code: 489

Topology: 4^6T44

# of independent nodes (IN): 6
Transitivity: [6(14)(12)4]
Space Group: C2
Pearson: mS20
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
4^6T44 (SACADA #489)		3.333		1.123	363.6	393.3	73.0	SACADA[1]
G198								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

10572.9760	592.1175	313.4958	0.0004	0.0000	196.1886
592.1175	8100.0774	2084.2270	0.0003	0.0003	-253.9490
313.4958	2084.2270	8100.1622	0.0001	0.0003	490.7902
0.0004	0.0003	0.0001	3788.2540	12.2187	0.0001
0.0000	0.0003	0.0003	12.2187	4141.0760	0.0002
196.1886	-253.9490	490.7902	0.0001	0.0002	4062.0895

[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].