SACADA Database Code: 488

Topology: 4^6T43

# of independent nodes (IN): 6
Transitivity: [6(14)(14)6]
Space Group: P2
Pearson: mP12
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
4^6T43 (SACADA #488)		3.491		0.944	397.3	462.5	87.3	SACADA[1]
G197								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

10984.1656	373.1110	510.0305	0.0000	-0.0000	-328.1400
373.1110	11548.5811	528.0441	0.0000	-0.0000	-27.2636
510.0305	528.0441	10424.9132	0.0000	0.0000	264.8283
0.0000	0.0000	0.0000	4738.0967	37.7531	0.0000
-0.0000	-0.0000	0.0000	37.7531	4049.0871	0.0000
-328.1400	-27.2636	264.8283	-0.0000	0.0000	3996.1033

[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].