SACADA Database Code: 419

Topology: 4^8T31

# of independent nodes (IN): 8
Transitivity: [8(16)(11)3]
Space Group: P21
Pearson: mP16
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
4^8T31 (SACADA #419)		3.418		0.924	387.2	439.6	82.6	SACADA[1]
G119								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

8743.3706	1087.9366	1452.6508	-0.0000	0.0000	132.2902
1087.9366	10840.8040	337.9966	-0.0000	-0.0000	-107.3307
1452.6508	337.9966	9545.4082	-0.0000	0.0000	189.1521
-0.0000	-0.0000	-0.0000	4784.3019	123.6974	0.0000
0.0000	-0.0000	0.0000	123.6974	4123.1076	0.0000
132.2902	-107.3307	189.1521	0.0000	0.0000	4445.4357

[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].