SACADA Database Code: 446

Topology: 4^6T38

# of independent nodes (IN): 6
Transitivity: [6(12)(12)6]
Space Group: P21
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
4^6T38 (SACADA #446)		3.203		1.022	359.5	336.2	57.6	SACADA[1]
G152								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

8594.4911	1774.3692	1386.4819	0.0000	0.0000	14.6105
1774.3692	8075.1844	636.9197	0.0000	0.0000	-213.5319
1386.4819	636.9197	8192.8578	-0.0000	-0.0000	-2.0080
-0.0000	0.0000	-0.0000	3961.7093	44.2644	-0.0000
0.0000	0.0000	-0.0000	44.2644	3130.1688	-0.0000
14.6105	-213.5319	-2.0080	-0.0000	-0.0000	2837.6168

[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].