SACADA Database Code: 516

Topology: 4^6T47

# of independent nodes (IN): 6
Transitivity: [6(15)(17)8]
Space Group: Pm
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
4^6T47 (SACADA #516)		3.183		0.965	355.4	330.7	56.4	SACADA[1]
G231								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

10414.8553	1025.7634	800.1966	-0.0000	-0.0000	21.1263
1025.7634	8340.9380	449.2038	-0.0000	-0.0000	206.3682
800.1966	449.2038	8873.5434	-0.0000	-0.0000	-126.5211
0.0000	0.0000	-0.0000	2395.4894	-348.5206	0.0000
-0.0000	-0.0000	-0.0000	-348.5206	2945.2972	-0.0000
21.1263	206.3682	-126.5211	0.0000	0.0000	3157.7073

[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].