SACADA Database Code: 377

Topology: 4^8T22

# of independent nodes (IN): 8
Transitivity: [(16)(28)(28)(16)]
Space Group: I2
Pearson: mS28
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
4^8T22 (SACADA #377)		3.440		0.859	402.5	453.0	85.0	SACADA[1]
G54								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

9255.6022	1450.9379	974.0722	0.0000	0.0000	-281.0164
1450.9379	9041.6208	1252.8461	0.0000	0.0001	-36.8156
974.0722	1252.8461	10616.7227	0.0000	0.0001	233.1239
0.0000	0.0000	0.0000	4664.9368	86.7627	0.0000
0.0000	0.0001	0.0001	86.7627	5142.6722	0.0000
-281.0164	-36.8156	233.1239	0.0000	0.0000	4534.9803

[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].