SACADA Database Code: 524

Topology: 4^2T286

# of independent nodes (IN): 2
Transitivity: [2763]
Space Group: P2/m
Pearson: mP8
Coordination Number (CN): 4

Year: 2019

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^2T286 (SACADA #524)		3.471		0.531	401.2	235.0	27.6	SACADA[1]
4,4T286		3.446	2.12		416	474	83	doi: 10.1038/s41598-019-42483-5

Elasticity tensor (kBar)[1]

11066.9373	-60.2056	422.6906	-0.0000	0.0000	237.9631
-60.2056	9723.8853	1308.4309	-0.0000	0.0000	-225.2180
422.6906	1308.4309	12230.7385	0.0000	-0.0000	62.3781
-0.0000	-0.0000	0.0000	3298.0999	353.4963	-0.0000
0.0000	0.0000	-0.0000	353.4963	4949.1337	-0.0000
237.9631	-225.2180	62.3781	-0.0000	0.0000	4802.2403

[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].