SACADA Database Code: 677

Topology: 4^4T46-CA

# of independent nodes (IN): 4
Transitivity: [4(10)61]
Space Group: P3221
Pearson: hP24
Coordination Number (CN): 4

Year: 2023

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^4T46-CA (SACADA #677)		3.283		0.499	346.4	376.8	70.0	SACADA[1]
4^4T46-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

7802.1100	1011.2916	930.1596	-0.0000	474.0768	-0.0000
1011.2916	7802.1100	930.1596	0.0000	-474.0768	0.0000
930.1596	930.1596	10010.0050	0.0000	0.0000	-0.0000
-0.0000	0.0000	0.0000	3395.4092	-0.0000	474.0768
474.0768	-474.0768	0.0000	-0.0000	4044.4874	0.0000
-0.0000	0.0000	-0.0000	474.0768	0.0000	4044.4873

[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].