SACADA Database Code: 671

Topology: 4^4T39-CA

# of independent nodes (IN): 4
Transitivity: [4982]
Space Group: I2/m
Pearson: mS24
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
4^4T39-CA (SACADA #671)		3.451		0.342	416.7	466.1	87.3	SACADA[1]
4^4T39-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

10849.1081	1000.7894	1145.2888	-0.0000	-0.0000	-111.3023
1000.7894	10729.7641	517.9587	-0.0000	-0.0000	437.6914
1145.2888	517.9587	10614.7434	-0.0000	-0.0000	8.5882
-0.0000	-0.0000	-0.0000	5165.7138	313.3247	-0.0000
-0.0000	-0.0000	-0.0000	313.3247	3814.1275	-0.0000
-111.3023	437.6914	8.5882	-0.0000	-0.0000	4620.9823

[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].