SACADA Database Code: 654

Topology: 4^4T1-CA

# of independent nodes (IN): 4
Transitivity: [4884]
Space Group: Pna21
Pearson: oP16
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
4^4T1-CA (SACADA #654)		3.507		0.447	424.6	479.0	89.9	SACADA[1]
4^4T1-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

10355.6941	889.9207	459.6975	0.0000	0.0000	0.0000
889.9207	11214.3216	738.6452	-0.0000	0.0000	0.0000
459.6975	738.6452	12568.7773	0.0000	0.0000	-0.0000
0.0000	0.0000	0.0000	3973.7075	-0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	5136.5614	-0.0000
0.0000	0.0000	-0.0000	-0.0000	0.0000	4358.6643

[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].