SACADA Database Code: 698

Topology: 4^4T71-CA

# of independent nodes (IN): 4
Transitivity: [4995]
Space Group: Pbcn
Pearson: oP32
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
4^4T71-CA (SACADA #698)		3.491		0.325	421.4	481.3	90.6	SACADA[1]
4^4T71-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

10724.8983	843.1027	917.7946	0.0000	-0.0000	-0.0000
843.1027	10355.1339	1110.2670	0.0000	0.0000	0.0000
917.7946	1110.2670	11123.3397	-0.0000	0.0000	-0.0000
-0.0000	0.0000	0.0000	4115.4995	0.0000	-0.0000
-0.0000	0.0000	0.0000	0.0000	4953.4429	0.0000
0.0000	0.0000	-0.0000	-0.0000	-0.0000	5309.1320

[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].