SACADA Database Code: 699

Topology: 4^4T73-CA

# of independent nodes (IN): 4
Transitivity: [4553]
Space Group: P6222
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
4^4T73-CA (SACADA #699)		3.624		1.396	428.4	410.0	71.6	SACADA[1]
4^4T73-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

10792.6079	1518.5689	713.2844	-0.0000	-0.0000	0.0000
1518.5689	10792.6079	713.2844	-0.0000	0.0000	-0.0000
713.2844	713.2844	11084.4170	-0.0000	0.0000	0.0000
-0.0000	-0.0000	-0.0000	4637.0195	-0.0000	-0.0000
-0.0000	0.0000	0.0000	-0.0000	3197.5192	-0.0000
0.0000	-0.0000	0.0000	-0.0000	-0.0000	3197.5192

[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].