SACADA Database Code: 695

Topology: 4^4T69-CA

# of independent nodes (IN): 4
Transitivity: [4(10)94]
Space Group: C2/c
Pearson: mS32
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
4^4T69-CA (SACADA #695)		3.441		0.547	395.0	435.0	81.2	SACADA[1]
4^4T69-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

9695.3533	212.2021	1555.0570	0.0000	-0.0000	782.4159
212.2021	11418.3470	466.4173	0.0000	-0.0000	219.2069
1555.0570	466.4173	9976.0359	0.0000	-0.0000	-331.9783
0.0000	0.0000	-0.0000	3728.4951	215.4948	-0.0000
-0.0000	-0.0000	-0.0000	215.4948	4244.1681	-0.0000
782.4159	219.2069	-331.9783	-0.0000	-0.0000	4337.7481

[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].