SACADA Database Code: 679

Topology: 4^4T50-CA

# of independent nodes (IN): 4
Transitivity: [49(10)5]
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
4^4T50-CA (SACADA #679)		3.512		0.648	405.6	440.4	81.8	SACADA[1]
4^4T50-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

12251.4755	550.8404	278.0195	0.0000	-0.0000	0.0000
550.8404	10531.9937	1172.2860	0.0000	-0.0000	-0.0000
278.0195	1172.2860	9800.5942	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	4130.7973	0.0000	-0.0000
-0.0000	-0.0000	-0.0000	0.0000	4153.9375	0.0000
0.0000	-0.0000	0.0000	-0.0000	0.0000	3763.6308

[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].