SACADA Database Code: 575

Topology: 4^3T150-CA

# of independent nodes (IN): 3
Transitivity: [39(10)4]
Space Group: I2/m
Pearson: mS24
Coordination Number (CN): 4

Year: 2021

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^3T150-CA (SACADA #575)		3.132		0.374	367.5	332.3	55.2	SACADA[1]
4^3T150-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

9959.5213	1927.4837	750.6820	-3.1362	1.8297	469.4684
1927.4837	7365.7941	1027.0085	3.4931	-5.1772	-246.6240
750.6820	1027.0085	8573.7871	17.9297	0.0062	250.4327
-3.1362	3.4931	17.9297	3295.5945	491.3381	7.8188
1.8297	-5.1772	0.0062	491.3381	2921.5037	1.9650
469.4684	-246.6240	250.4327	7.8188	1.9650	3157.5192

[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].