SACADA Database Code: 555

Topology: 4^3T51-CA

# of independent nodes (IN): 3
Transitivity: [39(10)6]
Space Group: Pnnn
Pearson: oP24
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
4^3T51-CA (SACADA #555)		3.421		0.534	399.0	419.8	77.2	SACADA[1]
4^3T51-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

11149.5236	99.3884	1066.1015	-0.0000	-0.0000	-0.0000
99.3884	11604.3167	602.7057	-0.0000	0.0000	-0.0000
1066.1015	602.7057	9656.9829	0.0000	0.0000	0.0000
-0.0000	-0.0000	0.0000	4145.2166	-0.0000	0.0000
-0.0000	0.0000	0.0000	-0.0000	3503.2406	-0.0000
0.0000	-0.0000	0.0000	0.0000	-0.0000	3476.4438

[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].