SACADA Database Code: 558

Topology: 4^3T55-CA

# of independent nodes (IN): 3
Transitivity: [3995]
Space Group: Pcca
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
4^3T55-CA (SACADA #558)		3.439		0.609	402.4	434.7	80.6	SACADA[1]
4^3T55-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

10675.9527	843.7397	866.6072	0.0000	0.0000	0.0000
843.7397	9494.9336	1084.6264	-0.0000	0.0000	0.0000
866.6072	1084.6264	10488.5590	0.0000	0.0000	0.0000
0.0000	-0.0000	0.0000	3868.2403	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	3916.8539	-0.0000
0.0000	0.0000	0.0000	0.0000	-0.0000	4764.5662

[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].