SACADA Database Code: 557

Topology: 4^3T53-CA

# of independent nodes (IN): 3
Transitivity: [3(10)(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
4^3T53-CA (SACADA #557)		3.320		0.538	386.0	399.1	72.8	SACADA[1]
4^3T53-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

10739.1700	267.0593	358.1217	0.0000	0.0000	-53.9709
267.0593	8549.2533	2242.6029	0.0000	0.0000	-263.4795
358.1217	2242.6029	9776.5518	0.0000	0.0000	55.8780
0.0000	0.0000	0.0000	3246.5336	159.6964	0.0000
0.0000	-0.0000	0.0000	159.6964	3966.7059	0.0000
-53.9709	-263.4795	55.8780	0.0000	0.0000	4313.4824

[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].