SACADA Database Code: 578

Topology: 4^3T153-CA

# of independent nodes (IN): 3
Transitivity: [3982]
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
4^3T153-CA (SACADA #578)		3.066		0.585	310.3	289.5	49.5	SACADA[1]
4^3T153-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

9240.8290	1032.2445	1485.3871	-1.5435	-0.8400	309.1641
1032.2445	4096.8261	1363.6326	-2.5896	0.1742	-155.4504
1485.3871	1363.6326	8772.0705	11.6308	-1.3660	434.6114
-1.5435	-2.5896	11.6308	2452.3514	363.9654	0.6626
-0.8400	0.1742	-1.3660	363.9654	2686.1436	0.9022
309.1641	-155.4504	434.6114	0.6626	0.9022	3873.8280

[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].