SACADA Database Code: 608

Topology: 4^3T185-CA

# of independent nodes (IN): 3
Transitivity: [3796]
Space Group: Imma
Pearson: oI32
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
4^3T185-CA (SACADA #608)		3.349		0.262	405.5	410.8	74.3	SACADA[1]
4^3T185-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

9132.8441	967.3990	849.8435	5.6789	1.2447	-0.4038
967.3990	10316.6101	1204.4731	-0.2516	-0.9316	0.4746
849.8435	1204.4731	11144.0271	1.5264	0.2850	0.4090
5.6789	-0.2516	1.5264	2961.9505	0.7988	-0.0521
1.2447	-0.9316	0.2850	0.7988	4810.9202	0.3319
-0.4038	0.4746	0.4090	-0.0521	0.3319	3924.2916

[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].