SACADA Database Code: 607

Topology: 4^3T184-CA

# of independent nodes (IN): 3
Transitivity: [3873]
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
4^3T184-CA (SACADA #607)		3.215		0.423	363.8	343.5	59.4	SACADA[1]
4^3T184-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

10061.8909	1083.0958	1245.6837	0.8087	-2.3209	-0.1028
1083.0958	6476.0346	1204.0548	1.5522	2.8041	-0.4028
1245.6837	1204.0548	9778.2216	8.8894	-0.4142	0.6193
0.8087	1.5522	8.8894	2699.0031	1.5340	0.3313
-2.3209	2.8041	-0.4142	1.5340	2950.4187	0.8050
-0.1028	-0.4028	0.6193	0.3313	0.8050	4337.2059

[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].