SACADA Database Code: 609

Topology: 4^3T186-CA

# of independent nodes (IN): 3
Transitivity: [3873]
Space Group: Immm
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
4^3T186-CA (SACADA #609)		3.225		0.441	361.5	358.1	64.0	SACADA[1]
4^3T186-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

9933.0515	1392.4526	967.2031	1.8954	-0.0696	0.7685
1392.4526	10166.8612	845.4086	-0.3168	-1.1407	-1.6782
967.2031	845.4086	6714.5027	5.5919	3.0084	0.1933
1.8954	-0.3168	5.5919	4159.8267	2.0497	-0.1942
-0.0696	-1.1407	3.0084	2.0497	3071.8690	2.1316
0.7685	-1.6782	0.1933	-0.1942	2.1316	3070.5425

[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].