SACADA Database Code: 606

Topology: 4^3T183-CA

# of independent nodes (IN): 3
Transitivity: [3775]
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
4^3T183-CA (SACADA #606)		3.256		0.520	356.8	314.4	50.7	SACADA[1]
4^3T183-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

10072.6718	1160.6684	1270.6224	-0.0000	0.0000	-0.0000
1160.6684	6539.0695	820.5951	0.0000	0.0000	-0.0000
1270.6224	820.5951	9647.0458	-0.0000	0.0000	-0.0000
0.0000	0.0000	-0.0000	2622.2707	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	1852.4867	0.0000
-0.0000	0.0000	-0.0000	0.0000	-0.0000	4471.6881

[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].