SACADA Database Code: 592

Topology: 4^3T168-CA

# of independent nodes (IN): 3
Transitivity: [3785]
Space Group: Pmma
Pearson: oP16
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
4^3T168-CA (SACADA #592)		3.229		0.425	370.0	299.1	42.8	SACADA[1]
4^3T168-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

10057.9790	992.8183	1253.9437	-0.0000	-0.0000	0.0000
992.8183	7131.1911	1063.7882	0.0000	-0.0000	-0.0000
1253.9437	1063.7882	9926.6664	0.0000	0.0000	0.0000
-0.0000	-0.0000	0.0000	1984.2649	0.0000	0.0000
-0.0000	-0.0000	0.0000	0.0000	1770.8222	0.0000
-0.0000	-0.0000	0.0000	-0.0000	0.0000	4424.0656

[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].