SACADA Database Code: 597

Topology: 4^3T173-CA

# of independent nodes (IN): 3
Transitivity: [3(10)(11)5]
Space Group: P42/nmc
Pearson: tP48
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
4^3T173-CA (SACADA #597)		2.742		0.906	268.6	184.1	21.3	SACADA[1]
4^3T173-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

4079.6722	1302.7307	1822.2847	0.0000	0.0000	-0.0000
1302.7307	4079.6722	1822.2847	0.0000	0.0000	-0.0000
1822.2847	1822.2847	7160.7173	0.0000	-0.0000	0.0000
0.0000	0.0000	0.0000	1806.1155	0.0000	0.0000
0.0000	-0.0000	-0.0000	0.0000	2060.9085	0.0000
0.0000	-0.0000	0.0000	0.0000	0.0000	2060.9085

[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].