SACADA Database Code: 594

Topology: 4^3T170-CA

# of independent nodes (IN): 3
Transitivity: [3(10)94]
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
4^3T170-CA (SACADA #594)		2.715		0.933	251.1	173.8	20.2	SACADA[1]
4^3T170-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

3655.9623	1179.5814	1767.4312	-0.0000	0.0000	0.0000
1179.5814	3655.9623	1767.4312	0.0000	-0.0000	-0.0000
1767.4312	1767.4312	7314.2891	-0.0000	0.0000	-0.0000
-0.0000	0.0000	0.0000	1610.0439	-0.0000	0.0000
0.0000	-0.0000	0.0000	0.0000	2020.5042	-0.0000
0.0000	-0.0000	-0.0000	0.0000	-0.0000	2020.5042

[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].