SACADA Database Code: 538

Topology: 4^2T38-CA

# of independent nodes (IN): 2
Transitivity: [2773]
Space Group: P42/nmc
Pearson: tP32
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
4^2T38-CA (SACADA #538)		3.089		0.481	353.4	301.9	46.8	SACADA[1]
4^2T38-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

6595.5847	1723.8856	1587.5362	0.0000	-0.0000	0.0000
1723.8856	6595.5847	1587.5362	0.0000	0.0000	0.0000
1587.5362	1587.5362	9087.5836	-0.0000	0.0000	-0.0000
-0.0000	0.0000	-0.0000	2597.4052	-0.0000	0.0000
-0.0000	0.0000	-0.0000	-0.0000	3449.4942	-0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	3449.4942

[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].