SACADA Database Code: 540

Topology: 4^2T39-CA

# of independent nodes (IN): 2
Transitivity: [2663]
Space Group: Immm
Pearson: oI24
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
4^2T39-CA (SACADA #540)		2.883		0.676	273.2	240.2	38.6	SACADA[1]
4^2T39-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

8009.1048	1341.0474	1365.5167	0.0000	0.0000	-0.0000
1341.0474	2701.6031	1669.4920	-0.0000	-0.0000	-0.0000
1365.5167	1669.4920	8342.8886	0.0000	-0.0000	0.0000
0.0000	-0.0000	0.0000	2173.6995	0.0000	0.0000
0.0000	-0.0000	0.0000	0.0000	2767.7938	0.0000
-0.0000	-0.0000	0.0000	0.0000	0.0000	3284.0808

[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].