SACADA Database Code: 542

Topology: 4^2T42-CA

# of independent nodes (IN): 2
Transitivity: [2774]
Space Group: I41/amd
Pearson: tI64
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
4^2T42-CA (SACADA #542)		2.778		0.971	250.1	158.4	18.0	SACADA[1]
4^2T42-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

3939.9015	1029.3476	1514.7582	0.0000	0.0000	0.0000
1029.3476	3939.9015	1514.7582	-0.0000	-0.0000	-0.0000
1514.7582	1514.7582	7821.6408	-0.0000	0.0000	0.0000
-0.0000	-0.0000	0.0000	1282.4715	0.0000	-0.0000
0.0000	-0.0000	0.0000	-0.0000	1505.1601	0.0000
-0.0000	-0.0000	0.0000	-0.0000	0.0000	1505.1601

[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].