SACADA Database Code: 543

Topology: 4^2T43-CA

# of independent nodes (IN): 2
Transitivity: [2563]
Space Group: I4/mcm
Pearson: tI32
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
4^2T43-CA (SACADA #543)		2.740		0.672	275.2	176.7	20.1	SACADA[1]
4^2T43-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

3607.0704	2673.5063	1107.7173	0.0000	0.0000	-0.0000
2673.5063	3607.0704	1107.7173	-0.0000	-0.0000	0.0000
1107.7173	1107.7173	8307.3111	-0.0000	-0.0000	-0.0000
0.0000	-0.0000	-0.0000	2282.7776	-0.0000	-0.0000
0.0000	-0.0000	-0.0000	-0.0000	2548.5373	0.0000
-0.0000	0.0000	-0.0000	-0.0000	0.0000	2548.5374

[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].