SACADA Database Code: 541

Topology: 4^2T40-CA

# of independent nodes (IN): 2
Transitivity: [2553]
Space Group: I-4m2
Pearson: tI24
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
4^2T40-CA (SACADA #541)		2.338		1.190	178.8	120.2	13.8	SACADA[1]
4^2T40-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

2122.0802	939.8379	1725.4696	-0.0000	0.0000	-0.0000
939.8379	2122.0802	1725.4696	0.0000	0.0000	0.0000
1725.4696	1725.4696	5474.6004	-0.0000	-0.0000	0.0000
-0.0000	0.0000	-0.0000	1129.4574	0.0000	0.0000
0.0000	0.0000	-0.0000	0.0000	1927.4910	0.0000
-0.0000	0.0000	-0.0000	0.0000	0.0000	1927.4910

[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].