SACADA Database Code: 529

Topology: 4^2T19-CA

# of independent nodes (IN): 2
Transitivity: [2641]
Space Group: Cmcm
Pearson: oS24
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
4^2T19-CA (SACADA #529)		3.269		0.308	392.1	383.1	67.8	SACADA[1]
4^2T19-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

9449.5803	1077.2033	1577.7862	0.0000	0.0000	0.0000
1077.2033	10630.3951	1378.1648	-0.0000	0.0000	-0.0000
1577.7862	1378.1648	7414.1101	0.0000	-0.0000	0.0000
0.0000	-0.0000	0.0000	4499.6819	0.0000	-0.0000
0.0000	0.0000	-0.0000	0.0000	4005.0614	-0.0000
0.0000	-0.0000	0.0000	-0.0000	-0.0000	3097.7682

[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].