SACADA Database Code: 545

Topology: 4^2T131

# of independent nodes (IN): 2
Transitivity: [2552]
Space Group: P42/nmc
Pearson: tP24
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
4^2T131 (SACADA #545)		2.974		0.612	326.5	266.0	38.5	SACADA[1]
4^2T131								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

5608.5837	1661.7569	1721.9494	4.7061	-1.2124	3.2933
1661.7569	5608.9199	1722.5440	1.2385	1.7798	-0.2241
1721.9494	1722.5440	8440.5105	8.1028	-0.6746	-0.3219
4.7061	1.2385	8.1028	2337.8439	0.7179	0.4511
-1.2124	1.7798	-0.6746	0.7179	3193.2447	3.7903
3.2933	-0.2241	-0.3219	0.4511	3.7903	3199.0839

[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].