SACADA Database Code: 604

Topology: 4^3T180-CA

# of independent nodes (IN): 3
Transitivity: [3(10)(10)4]
Space Group: Pmmn
Pearson: oP24
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
4^3T180-CA (SACADA #604)		2.704		0.902	252.3	197.6	26.9	SACADA[1]
4^3T180-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

2733.9838	1274.1607	1711.3932	0.0000	0.0000	0.0000
1274.1607	5282.0292	1924.5534	0.0000	-0.0000	0.0000
1711.3932	1924.5534	6991.2432	0.0000	0.0000	-0.0000
0.0000	0.0000	0.0000	2032.8115	-0.0000	-0.0000
0.0000	-0.0000	0.0000	-0.0000	2638.0553	-0.0000
0.0000	-0.0000	-0.0000	-0.0000	-0.0000	2471.3028

[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].