SACADA Database Code: 603

Topology: 4^3T179-CA

# of independent nodes (IN): 3
Transitivity: [3(10)93]
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
4^3T179-CA (SACADA #603)		3.170		0.402	369.0	338.4	57.0	SACADA[1]
4^3T179-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

9002.2081	1683.9187	937.4138	0.0000	0.0000	0.0000
1683.9187	5995.7311	1689.5412	-0.0000	-0.0000	-0.0000
937.4138	1689.5412	10112.3707	0.0000	-0.0000	-0.0000
0.0000	-0.0000	-0.0000	2766.3169	0.0000	-0.0000
0.0000	-0.0000	-0.0000	0.0000	3583.5910	-0.0000
0.0000	0.0000	-0.0000	0.0000	-0.0000	4042.1443

[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].