SACADA Database Code: 553

Topology: 4^3T49-CA

# of independent nodes (IN): 3
Transitivity: [3775]
Space Group: Immm
Pearson: oI24
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
4^3T49-CA (SACADA #553)		3.183		0.582	330.0	301.1	50.5	SACADA[1]
4^3T49-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

5852.3506	437.4327	629.2193	0.0000	0.0000	0.0000
437.4327	10319.7756	1741.9449	0.0000	-0.0000	-0.0000
629.2193	1741.9449	9158.0091	-0.0000	-0.0000	0.0000
0.0000	0.0000	-0.0000	2336.3532	-0.0000	0.0000
0.0000	-0.0000	-0.0000	-0.0000	3871.2996	-0.0000
0.0000	-0.0000	0.0000	0.0000	-0.0000	2033.1574

[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].