SACADA Database Code: 534

Topology: 4^2T34-CA

# of independent nodes (IN): 2
Transitivity: [2684]
Space Group: Cmmm
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
4^2T34-CA (SACADA #534)		3.181		0.405	370.8	319.4	50.1	SACADA[1]
4^2T34-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

9012.3992	888.4493	1676.8143	-0.0000	0.0000	0.0000
888.4493	10424.0242	1408.0715	-0.0000	-0.0000	0.0000
1676.8143	1408.0715	6415.2348	0.0000	-0.0000	-0.0000
-0.0000	-0.0000	0.0000	4078.9058	-0.0000	0.0000
0.0000	-0.0000	-0.0000	-0.0000	2543.3059	-0.0000
0.0000	-0.0000	-0.0000	0.0000	-0.0000	2553.0795

[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].