SACADA Database Code: 528

Topology: 4^2T18-CA

# of independent nodes (IN): 2
Transitivity: [2641]
Space Group: Cmcm
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
4^2T18-CA (SACADA #528)		2.693		0.945	253.4	216.8	33.7	SACADA[1]
4^2T18-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

6503.2422	2379.7540	1421.3543	0.0000	-0.0000	-0.0000
2379.7540	3977.5725	226.7048	-0.0000	0.0000	0.0000
1421.3543	226.7048	5573.7700	-0.0000	-0.0000	0.0000
0.0000	-0.0000	-0.0000	2485.1251	-0.0000	-0.0000
-0.0000	0.0000	0.0000	-0.0000	2330.1807	0.0000
-0.0000	0.0000	0.0000	-0.0000	0.0000	2459.5234

[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].