SACADA Database Code: 527

Topology: 4^2T17-CA

# of independent nodes (IN): 2
Transitivity: [2531]
Space Group: Pbcn
Pearson: oP16
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
4^2T17-CA (SACADA #527)		3.187		0.343	386.0	354.0	59.6	SACADA[1]
4^2T17-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

8358.9735	1312.0424	1505.5331	-0.0000	0.0000	-0.0000
1312.0424	10032.0530	835.7969	0.0000	0.0000	-0.0000
1505.5331	835.7969	9068.8748	0.0000	0.0000	-0.0000
-0.0000	-0.0000	0.0000	4557.1964	-0.0000	-0.0000
0.0000	0.0000	0.0000	-0.0000	3053.6536	0.0000
-0.0000	-0.0000	-0.0000	-0.0000	-0.0000	2572.2351

[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].