SACADA Database Code: 535

Topology: 4^2T35-CA

# of independent nodes (IN): 2
Transitivity: [2685]
Space Group: I41/amd
Pearson: tI64
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
4^2T35-CA (SACADA #535)		3.102		0.855	301.0	272.8	45.4	SACADA[1]
4^2T35-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

7337.0791	1626.4182	111.5885	6.8070	-0.7325	0.2053
1626.4182	7319.7933	113.4598	0.2482	2.5229	1.4320
111.5885	113.4598	8731.0678	9.0973	-1.6198	-2.1814
6.8070	0.2482	9.0973	1874.1290	5.1075	-2.8188
-0.7325	2.5229	-1.6198	5.1075	2539.7674	3.1757
0.2053	1.4320	-2.1814	-2.8188	3.1757	2544.4717

[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].