SACADA Database Code: 703

Topology: 4^3T16-CA

# of independent nodes (IN): 3
Transitivity: [3441]
Space Group: Ccca
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
4^3T16-CA (SACADA #703)		3.673		1.171	443.6	528.7	100.2	SACADA[1]
4^3T16-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

11539.1486	895.7510	951.1748	0.0000	-0.0000	0.0000
895.7510	12132.7171	532.1813	-0.0000	0.0000	-0.0000
951.1748	532.1813	11505.2421	0.0000	0.0000	0.0000
0.0000	-0.0000	0.0000	5287.0709	0.0000	-0.0000
-0.0000	0.0000	0.0000	0.0000	4880.5548	-0.0000
0.0000	-0.0000	0.0000	-0.0000	-0.0000	5361.9483

[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].