SACADA Database Code: 580

Topology: 4^3T155-CA

# of independent nodes (IN): 3
Transitivity: [3851]
Space Group: C2/c
Pearson: mS24
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
4^3T155-CA (SACADA #580)		3.327		0.329	403.6	436.6	81.0	SACADA[1]
4^3T155-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

9801.7137	1432.4830	749.6429	-0.0000	-0.0000	-19.7844
1432.4830	11358.9790	274.3186	-0.0000	-0.0000	151.3565
749.6429	274.3186	10320.5858	-0.0000	-0.0000	-381.3169
-0.0000	-0.0000	-0.0000	4241.0491	19.8249	-0.0000
-0.0000	-0.0000	-0.0000	19.8249	3736.9766	0.0000
-19.7844	151.3565	-381.3169	-0.0000	0.0000	4318.2999

[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].