SACADA Database Code: 530

Topology: 4^2T20-CA

# of independent nodes (IN): 2
Transitivity: [2652]
Space Group: C2/m
Pearson: mS12
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
4^2T20-CA (SACADA #530)		3.484		0.979	363.8	351.1	61.6	SACADA[1]
4^2T20-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

10573.9439	956.5568	49.7550	-0.0000	-0.0000	298.6454
956.5568	8402.0260	310.8346	0.0000	0.0000	-1090.8332
49.7550	310.8346	11276.4286	-0.0000	-0.0000	895.5237
-0.0000	0.0000	-0.0000	3005.4362	-1825.2878	0.0000
0.0000	0.0000	-0.0000	-1825.2878	2494.1452	0.0000
298.6454	-1090.8332	895.5237	0.0000	0.0000	3097.5142

[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].