SACADA Database Code: 539

Topology: 4^2T39

# of independent nodes (IN): 2
Transitivity: [2221]
Space Group: Ccca
Pearson: oS12
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
4^2T39 (SACADA #539)		3.657		1.256	436.5	510.4	96.5	SACADA[1]
4^2T39								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

12232.2756	887.2677	378.7116	-0.0000	0.0000	-0.0000
887.2677	11159.3381	1050.5618	0.0000	-0.0000	0.0000
378.7116	1050.5618	11281.5230	0.0000	-0.0000	0.0000
-0.0000	0.0000	0.0000	5049.3976	0.0000	-0.0000
0.0000	-0.0000	-0.0000	0.0000	5112.2194	-0.0000
-0.0000	0.0000	0.0000	-0.0000	-0.0000	4633.2663

[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].