SACADA Database Code: 622

Topology: sqc5270

# of independent nodes (IN): 2
Transitivity: [2442]
Space Group: I4/mmm
Pearson: tI24
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
sqc5270 (SACADA #622)		2.413		0.929	117.3	104.2	16.9	SACADA[1]
sqc5270								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

3871.4994	2716.9409	-123.6721	-0.0000	0.0000	-0.0000
2716.9409	3871.4994	-123.6721	0.0000	-0.0000	0.0000
-123.6721	-123.6721	8446.6401	0.0000	0.0000	-0.0000
-0.0000	-0.0000	0.0000	1119.8773	0.0000	-0.0000
0.0000	-0.0000	0.0000	0.0000	2362.1028	0.0000
-0.0000	0.0000	-0.0000	-0.0000	0.0000	2362.1028

[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].