SACADA Database Code: 616

Topology: cbs-4^2-Cmcm-2

# of independent nodes (IN): 2
Transitivity: [2553]
Space Group: Cmcm
Pearson: oS16
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
cbs-4^2-Cmcm-2 (SACADA #616)		3.071		0.757	337.5	280.5	41.9	SACADA[1]
cbs-4^2-Cmcm-2								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

8648.3268	941.8748	813.6351	0.0000	0.0000	0.0000
941.8748	11328.8353	1067.7806	0.0000	-0.0000	0.0000
813.6351	1067.7806	10406.8232	0.0000	0.0000	-0.0000
0.0000	0.0000	0.0000	3719.9442	0.0000	0.0000
0.0000	-0.0000	0.0000	0.0000	4874.7424	0.0000
0.0000	0.0000	-0.0000	0.0000	0.0000	3033.6879

[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].