SACADA Database Code: 619

Topology: cus

# of independent nodes (IN): 2
Transitivity: [2442]
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
cus (SACADA #619)		3.038		0.423	364.1	300.1	44.2	SACADA[1]
cus								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

9770.6093	864.2127	408.6641	0.0000	-0.0000	0.0000
864.2127	8289.0855	1444.7654	0.0000	0.0000	-0.0000
408.6641	1444.7654	9282.8567	-0.0000	-0.0000	-0.0000
0.0000	0.0000	-0.0000	3114.3793	0.0000	-0.0000
-0.0000	0.0000	-0.0000	0.0000	1441.8764	-0.0000
0.0000	-0.0000	-0.0000	-0.0000	-0.0000	3397.6188

[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].