SACADA Database Code: 629

Topology: umv

# of independent nodes (IN): 1
Transitivity: [1431]
Space Group: Fddd
Pearson: oF32
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
umv (SACADA #629)		3.000		0.977	293.1	133.6	18.2	SACADA[1]
umv								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

6574.4881	-487.9301	1332.7113	0.0000	-0.0000	0.0000
-487.9301	7195.8142	3198.5934	0.0000	0.0000	0.0000
1332.7113	3198.5934	4751.9337	-0.0000	0.0000	-0.0000
0.0000	0.0000	-0.0000	2612.6893	0.0000	0.0000
0.0000	-0.0000	0.0000	-0.0000	3425.7192	-0.0000
0.0000	0.0000	-0.0000	0.0000	-0.0000	2499.9520

[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].