SACADA Database Code: 630

Topology: yug

# of independent nodes (IN): 2
Transitivity: [2662]
Space Group: C2/m
Pearson: mS16
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
yug (SACADA #630)		2.979		0.500	344.4	286.8	42.9	SACADA[1]
yug								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

7559.0506	1393.1209	1187.0371	-0.0000	0.0000	-369.5642
1393.1209	7587.5314	1351.9956	0.0000	0.0000	-451.5603
1187.0371	1351.9956	7985.4075	-0.0000	0.0000	-182.6212
0.0000	0.0000	-0.0000	1812.5254	268.8018	0.0000
-0.0000	0.0000	0.0000	268.8018	2507.2939	0.0000
-369.5642	-451.5603	-182.6212	0.0000	0.0000	4183.7805

[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].