SACADA Database Code: 614

Topology: att

# of independent nodes (IN): 2
Transitivity: [2662]
Space Group: Pmma
Pearson: oP12
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
att (SACADA #614)		2.802		0.749	306.0	213.0	24.9	SACADA[1]
att								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

3977.8769	1708.2803	2212.1191	0.0000	-0.0000	0.0000
1708.2803	7027.2292	1709.0599	-0.0000	0.0000	-0.0000
2212.1191	1709.0599	5881.2873	0.0000	-0.0000	0.0000
-0.0000	-0.0000	0.0000	2398.2323	-0.0000	0.0000
-0.0000	0.0000	-0.0000	-0.0000	2061.5110	-0.0000
0.0000	-0.0000	0.0000	-0.0000	0.0000	2917.7769

[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].