SACADA Database Code: 621

Topology: sas

# of independent nodes (IN): 2
Transitivity: [2452]
Space Group: I4/mmm
Pearson: tI32
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
sas (SACADA #621)		2.500		0.746	273.4	207.6	26.9	SACADA[1]
sas								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

4454.6454	2616.9807	984.5847	0.0000	0.0000	-0.0000
2616.9807	4454.6454	984.5847	-0.0000	-0.0000	0.0000
984.5847	984.5847	6530.1463	-0.0000	-0.0000	0.0000
0.0000	-0.0000	-0.0000	3056.7662	0.0000	0.0000
-0.0000	-0.0000	-0.0000	0.0000	2321.2086	-0.0000
-0.0000	0.0000	0.0000	0.0000	0.0000	2321.2086

[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].