SACADA Database Code: 626

Topology: sta-4^2-P6422

# of independent nodes (IN): 2
Transitivity: [2222]
Space Group: P6222
Pearson: hP9
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
sta-4^2-P6422 (SACADA #626)		3.608		1.477	421.9	406.7	71.4	SACADA[1]
sta-4^2-P6422								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

10460.7245	1681.1744	707.3950	-0.0000	-0.0000	-0.0000
1681.1744	10460.7245	707.3950	0.0000	-0.0000	0.0000
707.3950	707.3950	10863.8888	-0.0000	0.0000	0.0000
-0.0000	0.0000	-0.0000	4389.7751	-0.0000	0.0000
-0.0000	-0.0000	0.0000	-0.0000	3340.2616	-0.0000
-0.0000	0.0000	0.0000	0.0000	-0.0000	3340.2616

[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].