SACADA Database Code: 140

Topology: 3,4T227

# of independent nodes (IN): 2
Transitivity: [2563]
Space Group: Cmcm
Pearson: oS24
Coordination Number (CN): 3, 4 (1:2)

Year: 2016

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
3,4T227 (SACADA #140)		3.171		0.329	367.0	329.4	54.2	SACADA[1]
oC24	52.8		1.29		371.4	340.4	51.7	doi: 10.1063/1.4952426

Elasticity tensor (kBar)[1]

10459.8786	775.9987	1604.5934	0.0000	0.0000	-0.0000
775.9987	6471.3897	713.2396	0.0000	-0.0000	0.0000
1604.5934	713.2396	11104.4933	-0.0000	-0.0000	0.0000
0.0000	0.0000	-0.0000	2024.9358	0.0000	-0.0000
0.0000	-0.0000	-0.0000	0.0000	2262.2730	-0.0000
-0.0000	0.0000	0.0000	-0.0000	-0.0000	5085.2537

[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].