SACADA Database Code: 359

Topology: 4^6T29

# of independent nodes (IN): 6
Transitivity: [6(13)(13)6]
Space Group: C2
Pearson: mS24
Coordination Number (CN): 4

Year: 2017

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^6T29 (SACADA #359)		3.530		0.819	421.4	497.5	94.2	SACADA[1]
G7								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

10952.4876	738.1587	528.4075	0.0000	0.0000	93.4738
738.1587	12116.1658	552.9464	-0.0000	0.0000	-7.0519
528.4075	552.9464	11254.1139	-0.0000	-0.0000	-243.3041
0.0000	-0.0000	-0.0000	5055.1617	-193.9497	-0.0000
0.0000	0.0000	-0.0000	-193.9497	4926.1188	0.0000
93.4738	-7.0519	-243.3041	-0.0000	0.0000	4181.7334

[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].