SACADA Database Code: 396

Topology: 4^8T26

# of independent nodes (IN): 8
Transitivity: [8(16)(11)3]
Space Group: P21
Pearson: mP16
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
4^8T26 (SACADA #396)		3.441		0.944	392.5	448.0	84.3	SACADA[1]
G87								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

11078.0732	391.2024	912.1709	0.0000	-0.0000	-126.4923
391.2024	10560.2528	877.4820	0.0000	-0.0000	-194.8666
912.1709	877.4820	9369.8566	0.0000	-0.0000	-221.9000
0.0000	0.0000	0.0000	4412.5467	-416.8966	-0.0000
-0.0000	-0.0000	-0.0000	-416.8966	4064.6447	0.0000
-126.4923	-194.8666	-221.9000	-0.0000	0.0000	4395.1681

[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].