SACADA Database Code: 285

Topology: 3^6,4T4

# of independent nodes (IN): 7
Transitivity: [7(16)(10)2]
Space Group: P21/m
Pearson: mP28
Coordination Number (CN): 3, 4 (6:1)

Year: 2013

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
3^6,4T4 (SACADA #285)		1.383		0.718	154.8	79.8	10.2	SACADA[1]
AGM-28		1.36	2.78					doi: 10.1002/adfm.201301077

Elasticity tensor (kBar)[1]

2089.2572	672.4367	1060.9639	-0.0000	0.0000	420.3607
672.4367	5625.9157	575.9125	0.0000	-0.0000	183.3019
1060.9639	575.9125	2341.9849	0.0000	0.0000	599.3893
-0.0000	0.0000	0.0000	1275.4136	473.1922	-0.0000
0.0000	-0.0000	0.0000	473.1922	1325.3434	-0.0000
420.3607	183.3019	599.3893	-0.0000	-0.0000	176.2225

[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].