SACADA Database Code: 249

Topology: 3^4,4T48

# of independent nodes (IN): 5
Transitivity: [5(12)82]
Space Group: P2/m
Pearson: mP20
Coordination Number (CN): 3, 4 (4:1)

Year: 2013

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
3^4,4T48 (SACADA #249)		1.722		0.784	191.1	96.2	12.4	SACADA[1]
AGM-20		1.70	2.78					doi: 10.1002/adfm.201301077

Elasticity tensor (kBar)[1]

2524.5910	901.3474	1279.6089	0.0000	0.0000	446.8339
901.3474	6587.9063	725.5192	-0.0000	0.0000	216.2897
1279.6089	725.5192	3119.3849	-0.0000	-0.0000	622.4901
-0.0000	0.0000	-0.0000	1551.3496	557.3656	0.0000
0.0000	0.0000	-0.0000	557.3656	1721.9257	-0.0000
446.8339	216.2897	622.4901	0.0000	-0.0000	193.0185

[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].