SACADA Database Code: 190

Topology: 3^2,4T97

# of independent nodes (IN): 3
Transitivity: [3862]
Space Group: P21/m
Pearson: mP12
Coordination Number (CN): 3, 4 (2:1)

Year: 2013

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
3^2,4T97 (SACADA #190)		2.260		0.947	250.6	125.4	16.3	SACADA[1]
AGM-12		2.23	1.66					doi: 10.1002/adfm.201301077

Elasticity tensor (kBar)[1]

3460.2939	1629.4777	1181.1349	-0.0000	-0.0000	445.5207
1629.4777	7052.5112	1223.1221	0.0000	-0.0000	272.9946
1181.1349	1223.1221	4884.7318	0.0000	0.0000	244.7797
-0.0000	0.0000	0.0000	1962.5185	531.0581	0.0000
-0.0000	-0.0000	0.0000	531.0581	2310.5100	0.0000
445.5207	272.9946	244.7797	0.0000	0.0000	262.6498

[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].