SACADA Database Code: 320

Topology: 3^9,4T1

# of independent nodes (IN): 10
Transitivity: -
Space Group: Cmmm
Pearson: oS56
Coordination Number (CN): 3, 4 (13:1)

Year: 2006

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
3^9,4T1 (SACADA #320)		.824		0.674	47.8	30.0	3.4	SACADA[1]
Zigzag carbon(5,5)					75.5	2.9		doi: 10.1103/PhysRevB.74.214104

Elasticity tensor (kBar)[1]

1718.8292	814.9865	406.2397	0.0000	-0.0000	0.0000
814.9865	386.7993	206.0815	-0.0000	0.0000	-0.0000
406.2397	206.0815	3635.2270	-0.0000	-0.0000	-0.0000
0.0000	-0.0000	-0.0000	40.9934	-0.0000	0.0000
-0.0000	0.0000	-0.0000	-0.0000	517.3060	0.0000
0.0000	-0.0000	-0.0000	0.0000	0.0000	993.7459

[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].