SACADA Database Code: 135

Topology: 4^2T109

# of independent nodes (IN): 2
Transitivity: [2543]
Space Group: C2
Pearson: mS8
Coordination Number (CN): 4

Year: 2004

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^2T109 (SACADA #135)		2.962		1.922	228.6	219.8	38.5	SACADA[1]
I		2.865	0.9		154.0			doi: 10.1103/PhysRevB.70.045101

Elasticity tensor (kBar)[1]

2864.4869	423.2384	1029.4305	0.0000	-0.0000	357.8953
423.2384	5362.3591	1751.4662	-0.0000	-0.0000	34.1083
1029.4305	1751.4662	8701.4748	-0.0000	-0.0000	1365.5557
0.0000	-0.0000	-0.0000	1752.8148	4.9789	-0.0000
-0.0000	-0.0000	-0.0000	4.9789	2855.7325	0.0000
357.8953	34.1083	1365.5557	-0.0000	0.0000	2355.4383

[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].