SACADA Database Code: 174

Topology: 4^3T83

# of independent nodes (IN): 3
Transitivity: [3552]
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
4^3T83 (SACADA #174)		2.978		1.396	342.1	282.3	41.7	SACADA[1]
F		2.950	0.6		297.4			doi: 10.1103/PhysRevB.70.045101

Elasticity tensor (kBar)[1]

6154.6679	1998.7431	1223.9878	-0.0000	0.0000	-259.9629
1998.7431	7439.5832	619.6140	0.0000	-0.0000	-524.6143
1223.9878	619.6140	9687.4096	-0.0000	0.0000	1783.2703
-0.0000	0.0000	-0.0000	2522.6848	933.2309	0.0000
0.0000	-0.0000	-0.0000	933.2309	2385.5568	0.0000
-259.9629	-524.6143	1783.2703	-0.0000	0.0000	3070.2881

[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].