SACADA Database Code: 175

Topology: 4^3T84

# of independent nodes (IN): 3
Transitivity: [3553]
Space Group: C2221
Pearson: oS16
Coordination Number (CN): 4

Year: 2011

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^3T84 (SACADA #175)		3.528		0.866	439.9	502.5	94.6	SACADA[1]
oC16-I			4.5		411.0		85.8	doi: 10.1103/PhysRevB.84.161411
oC16-I								doi: 10.3103/s1063457613010012
oC16-I								doi: 10.1002/zaac.201300652

Elasticity tensor (kBar)[1]

10079.1557	1939.4233	864.1294	-0.0000	-0.0000	-0.0000
1939.4233	9870.8607	718.1096	0.0000	0.0000	0.0000
864.1294	718.1096	12669.8342	-0.0000	-0.0000	-0.0000
-0.0000	0.0000	-0.0000	5232.3446	-0.0000	-0.0000
-0.0000	0.0000	-0.0000	-0.0000	4867.0586	0.0000
-0.0000	0.0000	-0.0000	-0.0000	0.0000	5529.1076

[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].