SACADA Database Code: 247

Topology: 4^5T14

# of independent nodes (IN): 5
Transitivity: [5984]
Space Group: I2/m
Pearson: mS20
Coordination Number (CN): 4

Year: 2013

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^5T14 (SACADA #247)		3.424		0.719	422.2	459.4	85.4	SACADA[1]
C2/m-20	25.0	3.374					85.9	doi: 10.1063/1.4794424
C2/m-20								doi: 10.1039/c6ra02081j

Elasticity tensor (kBar)[1]

11620.1468	683.5957	1239.4204	0.0000	0.0000	206.8280
683.5957	11328.1057	868.8551	0.0000	-0.0000	-237.3128
1239.4204	868.8551	9562.5694	-0.0000	0.0000	-148.3670
0.0000	0.0000	-0.0000	5057.3560	-530.4435	0.0000
0.0000	-0.0000	0.0000	-530.4435	4209.8858	0.0000
206.8280	-237.3128	-148.3670	0.0000	0.0000	3957.7700

[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].