SACADA Database Code: 186

Topology: 4^3T85

# of independent nodes (IN): 3
Transitivity: [3763]
Space Group: C2/m
Pearson: mS16
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
4^3T85 (SACADA #186)		3.394		0.775	417.0	461.2	86.1	SACADA[1]
C2/m-16	0-100	3.344	4.197		398	458	84.9	doi: 10.1063/1.4794424
C2/m-16								doi: 10.1007/s10853-015-9266-8
C2/m-16								doi: 10.1039/c6ra02081j

Elasticity tensor (kBar)[1]

10681.4697	303.3818	957.9032	3.1601	-0.0421	-20.3467
303.3818	10530.8368	1430.2272	2.1774	0.8322	-167.6358
957.9032	1430.2272	10995.7214	5.8199	-0.3364	-48.6610
3.1601	2.1774	5.8199	3715.9672	-152.3788	0.3950
-0.0421	0.8322	-0.3364	-152.3788	5185.4398	2.6747
-20.3467	-167.6358	-48.6610	0.3950	2.6747	4501.1450

[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].