SACADA Database Code: 144

Topology: 4^2T110

# of independent nodes (IN): 2
Transitivity: [2773]
Space Group: Cmcm
Pearson: oS32
Coordination Number (CN): 4

Year: 2012

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^2T110 (SACADA #144)		3.450		0.699	430.0	478.8	89.6	SACADA[1]
A4-A2B2		3.397	3.271		413.62		83.18	doi: 10.3103/s1063457612060123
A4-A2B2								doi: 10.1039/c2cp40531h
Cmca								doi: 10.1103/PhysRevB.91.214104

Elasticity tensor (kBar)[1]

11209.3783	718.5051	452.9481	0.0000	-0.0000	0.0000
718.5051	11164.6043	1127.3640	-0.0000	-0.0000	0.0000
452.9481	1127.3640	11743.3006	-0.0000	0.0000	-0.0000
0.0000	0.0000	-0.0000	3874.9735	-0.0000	0.0000
-0.0000	0.0000	0.0000	0.0000	5226.4728	0.0000
0.0000	-0.0000	0.0000	0.0000	0.0000	4432.0783

[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].