SACADA Database Code: 292

Topology: 4^8T14

# of independent nodes (IN): 8
Transitivity: [8(14)(12)7]
Space Group: C2/m
Pearson: mS32
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
4^8T14 (SACADA #292)		3.461		0.653	434.6	494.2	92.9	SACADA[1]
16A	20							doi: 10.1103/PhysRevB.88.014102

Elasticity tensor (kBar)[1]

10595.3651	502.3917	1653.8895	0.0000	0.0000	867.1698
502.3917	11680.1911	865.0513	0.0000	-0.0000	-394.2846
1653.8895	865.0513	10805.5719	-0.0000	0.0000	-155.3538
0.0000	0.0000	-0.0000	4387.3589	-369.4464	0.0000
0.0000	-0.0000	0.0000	-369.4464	5270.2864	0.0000
867.1698	-394.2846	-155.3538	0.0000	0.0000	5131.5636

[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].