SACADA Database Code: 268

Topology: 4^6T13

# of independent nodes (IN): 6
Transitivity: [6(13)(15)(11)]
Space Group: Pmmn
Pearson: oP24
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
4^6T13 (SACADA #268)		3.481		0.662	436.9	492.5	92.4	SACADA[1]
B-B1AL0R4	6.7	3.54			454.9	502.3	82.4	doi: 10.1103/PhysRevLett.108.135501

Elasticity tensor (kBar)[1]

12196.5910	305.1095	984.0729	0.0000	-0.0000	0.0000
305.1095	11844.3802	723.8904	-0.0000	-0.0000	-0.0000
984.0729	723.8904	11266.1545	-0.0000	0.0000	-0.0000
0.0000	-0.0000	-0.0000	4607.0505	-0.0000	-0.0000
-0.0000	-0.0000	0.0000	-0.0000	3925.2003	-0.0000
0.0000	-0.0000	-0.0000	-0.0000	-0.0000	5227.5367

[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].