SACADA Database Code: 269

Topology: 4^6T14

# of independent nodes (IN): 6
Transitivity: [6(13)(16)(11)]
Space Group: Pmma
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
4^6T14 (SACADA #269)		3.482		0.664	436.9	492.8	92.5	SACADA[1]
B-B1AL1R3	6.4	3.54			456.2	505.3	83.0	doi: 10.1103/PhysRevLett.108.135501

Elasticity tensor (kBar)[1]

11987.2286	276.1718	613.6985	0.0000	-0.0000	0.0000
276.1718	12172.7977	1007.9184	0.0000	0.0000	-0.0000
613.6985	1007.9184	11370.9504	-0.0000	0.0000	-0.0000
0.0000	0.0000	-0.0000	4594.1661	0.0000	-0.0000
-0.0000	0.0000	0.0000	0.0000	5247.6458	0.0000
-0.0000	0.0000	-0.0000	-0.0000	0.0000	3852.6462

[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 2π × 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].