SACADA Database Code: 189

Topology: 4^3T129

# of independent nodes (IN): 3
Transitivity: [3797]
Space Group: Immm
Pearson: oI24
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
4^3T129 (SACADA #189)		3.482		0.664	436.9	492.5	92.4	SACADA[1]
B-B1AL2R2	20	3.54			456.3	504.4	82.7	doi: 10.1103/PhysRevLett.108.135501
12A								doi: 10.1103/PhysRevB.88.014102

Elasticity tensor (kBar)[1]

11374.4603	1001.0987	617.1863	0.0000	-0.0000	-0.0000
1001.0987	12174.8180	282.8895	-0.0000	0.0000	0.0000
617.1863	282.8895	11980.2246	0.0000	-0.0000	-0.0000
0.0000	-0.0000	0.0000	5246.2250	-0.0000	0.0000
-0.0000	0.0000	-0.0000	-0.0000	4589.4292	0.0000
0.0000	0.0000	-0.0000	0.0000	0.0000	3846.7859

[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].