SACADA Database Code: 134

Topology: cbs-3,4-Pnma

# of independent nodes (IN): 2
Transitivity: [2542]
Space Group: Cmcm
Pearson: oS16
Coordination Number (CN): 3, 4 (1:1)

Year: 2011

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
cbs-3,4-Pnma (SACADA #134)		3.128		0.253	351.2	281.2	39.6	SACADA[1]
3D-(5,0)		3.20			352.5	285.5	40.9	doi: 10.1021/nn202053t
mC16-carbon								doi: 10.3103/s1063457614040042

Elasticity tensor (kBar)[1]

5545.6792	650.9021	52.0305	0.0000	0.0000	0.0000
650.9021	11877.3498	1536.1102	-0.0000	0.0000	-0.0000
52.0305	1536.1102	12281.2807	0.0000	-0.0000	-0.0000
0.0000	-0.0000	0.0000	979.0191	-0.0000	-0.0000
0.0000	-0.0000	0.0000	-0.0000	4959.3899	0.0000
0.0000	-0.0000	-0.0000	0.0000	0.0000	1892.5621

[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].