SACADA Database Code: 146

Topology: 4^2T113

# of independent nodes (IN): 2
Transitivity: [2784]
Space Group: Cccm
Pearson: oS32
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
4^2T113 (SACADA #146)		3.284		0.885	397.1	403.9	73.1	SACADA[1]
3D (4,0)-III	35				398.7	416.3	91.9	doi: 10.1038/srep01331

Elasticity tensor (kBar)[1]

9491.1459	2068.4065	767.8027	0.0000	0.0000	0.0000
2068.4065	8807.4193	498.6880	-0.0000	-0.0000	0.0000
767.8027	498.6880	10804.7328	0.0000	-0.0000	0.0000
0.0000	-0.0000	-0.0000	4383.5360	0.0000	0.0000
0.0000	-0.0000	-0.0000	0.0000	3907.5507	0.0000
0.0000	0.0000	-0.0000	0.0000	0.0000	3509.1453

[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].