SACADA Database Code: 275

Topology: 4^7T15

# of independent nodes (IN): 7
Transitivity: [7(10)(10)7]
Space Group: Imma
Pearson: oI40
Coordination Number (CN): 4

Year: 2016

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^7T15 (SACADA #275)		3.473		0.638	431.0	491.2	92.4	SACADA[1]
4(II)			4.139(D)					doi: 10.1103/PhysRevB.93.085201

Elasticity tensor (kBar)[1]

11504.5986	295.0380	1255.9076	0.0000	-0.0000	0.0000
295.0380	10955.6830	1403.1900	0.0000	0.0000	-0.0000
1255.9076	1403.1900	10424.2673	-0.0000	0.0000	0.0000
0.0000	0.0000	-0.0000	4262.0661	0.0000	0.0000
-0.0000	-0.0000	0.0000	0.0000	5059.6929	-0.0000
0.0000	-0.0000	0.0000	0.0000	-0.0000	5386.3444

[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].