SACADA Database Code: 131

Topology: lib-3,4-P42/mmc

# of independent nodes (IN): 2
Transitivity: [2453]
Space Group: P42/mmc
Pearson: tP12
Coordination Number (CN): 3, 4 (1:2)

Year: 2013

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
lib-3,4-P42/mmc (SACADA #131)		2.533		0.891	298.6	218.1	26.8	SACADA[1]
3D (6,0)-I			0.69		298.63	231.11	81.07	doi: 10.1038/srep01331

Elasticity tensor (kBar)[1]

7238.1232	303.6434	499.4909	-0.0000	-0.0000	0.0000
303.6434	7238.1232	499.4909	0.0000	0.0000	-0.0000
499.4909	499.4909	10176.7362	0.0000	-0.0000	-0.0000
-0.0000	0.0000	0.0000	480.4849	-0.0000	0.0000
0.0000	0.0000	-0.0000	-0.0000	2967.6420	0.0000
0.0000	-0.0000	-0.0000	0.0000	0.0000	2967.6420

[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].