SACADA Database Code: 366

Topology: 4^3T170

# of independent nodes (IN): 3
Transitivity: [3664]
Space Group: Imma
Pearson: oI20
Coordination Number (CN): 4

Year: 2017

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^3T170 (SACADA #366)		3.344		0.794	382.9	432.1	81.1	SACADA[1]
G22								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

10917.6766	73.6796	1068.6332	-0.0000	-0.0000	0.0000
73.6796	11811.2797	183.9960	0.0000	-0.0000	-0.0000
1068.6332	183.9960	9177.4747	-0.0000	0.0000	0.0000
-0.0000	0.0000	-0.0000	4133.3128	0.0000	0.0000
-0.0000	-0.0000	0.0000	0.0000	2958.0667	0.0000
0.0000	-0.0000	0.0000	0.0000	0.0000	4854.1721

[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].