SACADA Database Code: 374

Topology: 4^3T172

# of independent nodes (IN): 3
Transitivity: [3442]
Space Group: I222
Pearson: oI14
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
4^3T172 (SACADA #374)		3.157		1.161	333.2	330.0	58.9	SACADA[1]
G47								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

7757.0206	938.6585	862.8554	-0.0000	-0.0000	-0.0000
938.6585	9191.3854	1091.7260	0.0000	-0.0000	0.0000
862.8554	1091.7260	7396.1404	-0.0000	-0.0000	-0.0000
0.0000	0.0000	-0.0000	4079.5246	-0.0000	-0.0000
-0.0000	-0.0000	-0.0000	0.0000	1987.6145	0.0000
-0.0000	0.0000	-0.0000	-0.0000	0.0000	3865.7349

[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].