SACADA Database Code: 372

Topology: 4^3T171

# of independent nodes (IN): 3
Transitivity: [3873]
Space Group: C2/c
Pearson: mS20
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
4^3T171 (SACADA #372)		3.469		0.954	389.4	445.8	83.9	SACADA[1]
G39								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

9215.6483	1478.4259	853.0317	-0.0000	-0.0000	341.2105
1478.4259	9243.6174	217.7511	0.0000	-0.0000	-391.2393
853.0317	217.7511	11560.4820	-0.0000	-0.0000	191.1453
-0.0000	-0.0000	-0.0000	4250.6807	-184.9006	-0.0000
0.0000	-0.0000	-0.0000	-184.9006	4002.1567	-0.0000
341.2105	-391.2393	191.1453	-0.0000	-0.0000	5070.6909

[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].