SACADA Database Code: 471

Topology: 4^5T60

# of independent nodes (IN): 5
Transitivity: [5(12)(12)6]
Space Group: Amm2
Pearson: oS32
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
4^5T60 (SACADA #471)		3.288		0.900	374.2	377.5	68.1	SACADA[1]
G179								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

9267.3566	414.7150	804.0927	0.0000	0.0000	-0.0000
414.7150	9747.5833	1185.5276	-0.0000	0.0000	-0.0000
804.0927	1185.5276	9910.0588	0.0000	0.0000	0.0000
0.0000	-0.0000	-0.0000	3306.4956	0.0000	0.0000
-0.0000	0.0000	-0.0000	0.0000	4099.5992	0.0000
-0.0000	-0.0000	0.0000	-0.0000	0.0000	2904.9056

[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].