SACADA Database Code: 428

Topology: 4^5T58

# of independent nodes (IN): 5
Transitivity: [5(12)(10)4]
Space Group: C2/m
Pearson: mS32
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
4^5T58 (SACADA #428)		3.389		0.753	400.5	446.6	83.6	SACADA[1]
G128								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

9958.6052	355.0051	1119.1466	-0.0000	-0.0000	18.3352
355.0051	10419.2712	1149.1403	0.0000	0.0000	-41.2956
1119.1466	1149.1403	10469.3414	0.0000	0.0000	-53.5405
-0.0000	0.0000	0.0000	3706.1347	-57.5577	-0.0000
-0.0000	0.0000	0.0000	-57.5577	4928.6984	-0.0000
18.3352	-41.2956	-53.5405	-0.0000	-0.0000	4414.0000

[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].