SACADA Database Code: 423

Topology: 4^5T57

# of independent nodes (IN): 5
Transitivity: [5995]
Space Group: C2221
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
4^5T57 (SACADA #423)		3.413		0.904	388.2	440.0	82.7	SACADA[1]
G123								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

8893.7023	1324.5970	1355.1973	-0.0000	0.0000	-0.0000
1324.5970	9330.2666	769.9654	-0.0000	-0.0000	-0.0000
1355.1973	769.9654	9821.3108	-0.0000	-0.0000	-0.0000
-0.0000	-0.0000	-0.0000	4698.3434	0.0000	-0.0000
0.0000	-0.0000	-0.0000	0.0000	4279.5173	-0.0000
-0.0000	-0.0000	-0.0000	-0.0000	-0.0000	4910.4982

[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].