SACADA Database Code: 411

Topology: 4^4T115

# of independent nodes (IN): 4
Transitivity: [4643]
Space Group: Pmmn
Pearson: oP12
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
4^4T115 (SACADA #411)		3.264		0.816	380.0	430.8	80.9	SACADA[1]
G105								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

10578.2245	776.9032	335.5600	-0.0000	-0.0000	0.0000
776.9032	8484.5137	1230.7441	0.0000	-0.0000	-0.0000
335.5600	1230.7441	10534.7555	0.0000	0.0000	0.0000
-0.0000	0.0000	0.0000	4591.1132	-0.0000	0.0000
-0.0000	-0.0000	-0.0000	-0.0000	3723.3578	-0.0000
0.0000	-0.0000	0.0000	0.0000	-0.0000	4286.5439

[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].