SACADA Database Code: 491

Topology: 4^3T186

# of independent nodes (IN): 3
Transitivity: [3553]
Space Group: C222
Pearson: oS14
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
4^3T186 (SACADA #491)		3.564		1.254	391.8	448.0	84.3	SACADA[1]
G201								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

11687.5223	393.9200	531.9427	0.0000	-0.0000	0.0109
393.9200	10223.5060	1479.9926	0.0000	0.0000	0.0010
531.9427	1479.9926	8650.7861	0.0000	0.0000	0.0091
0.0000	0.0000	0.0000	4338.5140	0.0049	0.0000
-0.0000	-0.0000	0.0000	0.0049	4886.1897	0.0000
0.0109	0.0010	0.0091	0.0000	-0.0000	3978.6845

[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].