SACADA Database Code: 367

Topology: 4^4T110

# of independent nodes (IN): 4
Transitivity: [4774]
Space Group: C2221
Pearson: oS24
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
4^4T110 (SACADA #367)		3.441		0.852	410.0	451.2	84.2	SACADA[1]
G24								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

8928.8610	1530.5518	1191.8041	0.0000	-0.0000	0.0000
1530.5518	9220.7585	964.0630	0.0000	-0.0000	0.0000
1191.8041	964.0630	11512.0840	-0.0000	0.0000	-0.0000
0.0000	0.0000	0.0000	4425.6400	0.0000	-0.0000
-0.0000	-0.0000	0.0000	0.0000	4529.1118	0.0000
0.0000	0.0000	-0.0000	-0.0000	0.0000	5086.6899

[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].