SACADA Database Code: 369

Topology: 4^4T111

# of independent nodes (IN): 4
Transitivity: [4664]
Space Group: I212121
Pearson: oI20
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
4^4T111 (SACADA #369)		3.413		0.832	404.7	440.2	81.8	SACADA[1]
G27								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

8969.8356	1231.2068	1532.1107	-0.0000	0.0000	-0.0000
1231.2068	10814.9386	637.1528	0.0000	-0.0000	-0.0000
1532.1107	637.1528	9867.3419	0.0000	0.0000	-0.0000
0.0000	-0.0000	0.0000	5238.3955	0.0000	0.0000
0.0000	-0.0000	0.0000	0.0000	3716.9987	0.0000
-0.0000	-0.0000	-0.0000	0.0000	0.0000	4503.8938

[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].