SACADA Database Code: 393

Topology: 4^4T113

# of independent nodes (IN): 4
Transitivity: [4994]
Space Group: Fdd2
Pearson: oF64
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
4^4T113 (SACADA #393)		3.468		1.084	396.0	435.8	81.3	SACADA[1]
G84								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

10589.8466	620.2691	1236.1305	0.0000	0.0000	-0.0000
620.2691	10900.7634	428.2436	-0.0000	-0.0000	0.0000
1236.1305	428.2436	9620.9152	0.0000	-0.0000	0.0000
0.0000	-0.0000	0.0000	4277.9574	0.0000	-0.0000
0.0000	-0.0000	-0.0000	0.0000	3421.3130	-0.0000
-0.0000	0.0000	0.0000	-0.0000	-0.0000	4692.9686

[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].