SACADA Database Code: 517

Topology: 4^2T267

# of independent nodes (IN): 2
Transitivity: [2795]
Space Group: Ibam
Pearson: oI32
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
4^2T267 (SACADA #517)		3.370		0.793	396.1	441.5	82.6	SACADA[1]
G234								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

8761.5881	1890.8000	98.4755	-0.0000	-0.0000	-0.0000
1890.8000	10289.3041	157.9159	-0.0000	-0.0000	-0.0000
98.4755	157.9159	12429.7589	-0.0000	0.0000	-0.0000
-0.0000	-0.0000	-0.0000	4489.7018	-0.0000	0.0000
-0.0000	0.0000	0.0000	0.0000	4210.6803	0.0000
-0.0000	-0.0000	0.0000	0.0000	0.0000	3901.2728

[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].