SACADA Database Code: 386

Topology: 4^4T112

# of independent nodes (IN): 4
Transitivity: [4994]
Space Group: I2
Pearson: mS16
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
4^4T112 (SACADA #386)		3.490		1.003	400.4	459.9	86.7	SACADA[1]
G72								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

9835.9146	433.2156	1273.7435	-0.0000	-0.0000	549.1300
433.2156	11989.0205	598.5918	0.0000	0.0000	16.2391
1273.7435	598.5918	9664.3321	0.0000	0.0000	-678.0394
-0.0000	0.0000	0.0000	4181.8923	-97.3911	0.0000
-0.0000	0.0000	0.0000	-97.3911	4860.3842	0.0000
549.1300	16.2391	-678.0394	-0.0000	0.0000	4354.3997

[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].