SACADA Database Code: 358

Topology: 4^6T28

# of independent nodes (IN): 6
Transitivity: [6875]
Space Group: Imm2
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
4^6T28 (SACADA #358)		3.376		0.705	403.1	455.2	85.4	SACADA[1]
G6								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

10958.7096	329.8802	839.5792	-0.0000	0.0000	0.0000
329.8802	11154.2277	1014.8566	0.0000	-0.0000	0.0000
839.5792	1014.8566	9817.4100	-0.0000	0.0000	0.0000
-0.0000	0.0000	-0.0000	4338.2107	-0.0000	0.0000
0.0000	-0.0000	0.0000	-0.0000	3862.1820	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	4778.7254

[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].