SACADA Database Code: 282

Topology: 4^7T7

# of independent nodes (IN): 7
Transitivity: [7(12)(11)6]
Space Group: I2/m
Pearson: mS28
Coordination Number (CN): 4

Year: 2013

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^7T7 (SACADA #282)		3.421		0.670	424.5	476.5	89.3	SACADA[1]
14A	20							doi: 10.1103/PhysRevB.88.014102

Elasticity tensor (kBar)[1]

11159.2846	757.2777	1113.0529	-0.0000	-0.0000	-606.5329
757.2777	11320.2651	802.1473	-0.0000	-0.0000	384.9352
1113.0529	802.1473	10397.3577	0.0000	0.0000	236.9641
-0.0000	-0.0000	0.0000	4942.7125	513.8602	-0.0000
-0.0000	-0.0000	0.0000	513.8602	4679.8316	-0.0000
-606.5329	384.9352	236.9641	-0.0000	-0.0000	4203.3673

[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].