SACADA Database Code: 281

Topology: 4^7T8

# of independent nodes (IN): 7
Transitivity: [7(12)(11)6]
Space Group: C2/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
4^7T8 (SACADA #281)		3.459		0.697	426.9	476.3	89.2	SACADA[1]
14C	20							doi: 10.1103/PhysRevB.88.014102

Elasticity tensor (kBar)[1]

9679.5187	684.5985	1483.0047	-0.0000	0.0000	-15.8002
684.5985	11426.9638	975.1953	-0.0000	0.0000	-296.8689
1483.0047	975.1953	11111.8918	0.0000	-0.0000	667.1988
-0.0000	-0.0000	0.0000	4136.5842	-181.0328	-0.0000
0.0000	0.0000	-0.0000	-181.0328	5431.5330	0.0000
-15.8002	-296.8689	667.1988	-0.0000	0.0000	4688.0489

[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].