SACADA Database Code: 347

Topology: 4^{20}T2

# of independent nodes (IN): 20
Transitivity: [(20)(30)(28)(18)]
Space Group: Pm
Pearson: mP20
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^{20}T2 (SACADA #347)		3.476		0.653	416.5	484.5	91.5	SACADA[1]
20B	20							doi: 10.1103/PhysRevB.88.014102

Elasticity tensor (kBar)[1]

10683.2323	439.0584	790.5669	0.0000	-0.0000	292.2159
439.0584	11258.0499	896.3204	0.0000	0.0000	-269.6932
790.5669	896.3204	11322.2016	-0.0000	0.0000	-106.1034
0.0000	0.0000	-0.0000	4242.6685	-326.6382	0.0000
-0.0000	0.0000	0.0000	-326.6382	5178.1421	-0.0000
292.2159	-269.6932	-106.1034	0.0000	-0.0000	4517.2447

[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].