SACADA Database Code: 348

Topology: 4^{20}T3

# of independent nodes (IN): 14
Transitivity: [(20)(32)(31)(19)]
Space Group: P2/m
Pearson: mP40
Coordination Number (CN): 4

Year: 2016

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^{20}T3 (SACADA #348)		3.509		0.604	422.9	495.0	93.6	SACADA[1]
9								doi: 10.1103/PhysRevB.93.085201

Elasticity tensor (kBar)[1]

10938.3039	277.5434	1261.0313	0.0000	0.0000	1.7360
277.5434	11281.9437	1221.0794	-0.0000	-0.0000	0.3294
1261.0313	1221.0794	10320.6970	-0.0000	-0.0000	9.1574
0.0000	-0.0000	-0.0000	4372.1880	0.0980	-0.0000
0.0000	-0.0000	-0.0000	0.0980	5397.7225	-0.0000
1.7360	0.3294	9.1574	-0.0000	-0.0000	5160.0694

[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].