SACADA Database Code: 97

Topology: 4^2T111

# of independent nodes (IN): 2
Transitivity: [2232]
Space Group: I-42d
Pearson: tI12
Coordination Number (CN): 4

Year: 2011

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^2T111 (SACADA #97)		3.699		1.108	447.3	563.1	107.4	SACADA[1]
tI12			4.1		425.0		87.2	doi: 10.1103/PhysRevB.83.193410
tI12								link
tI12								doi: 10.3103/s1063457613010012

Elasticity tensor (kBar)[1]

11762.4928	577.8491	872.3040	0.0000	-0.0000	0.0000
577.8491	11762.4928	872.3040	0.0000	0.0000	-0.0000
872.3040	872.3040	12099.8818	-0.0000	0.0000	-0.0000
0.0000	0.0000	-0.0000	5349.9455	-0.0000	-0.0000
-0.0000	0.0000	-0.0000	-0.0000	5862.5085	-0.0000
0.0000	-0.0000	0.0000	-0.0000	0.0000	5862.5086

[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].