SACADA Database Code: 138

Topology: 3,4T90

# of independent nodes (IN): 2
Transitivity: [2562]
Space Group: I2/m
Pearson: mS12
Coordination Number (CN): 3, 4 (1:2)

Year: 2016

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
3,4T90 (SACADA #138)		3.170		0.330	368.8	330.3	54.3	SACADA[1]
mC12			1.07		371.4	339.8	51.5	doi: 10.1063/1.4952426

Elasticity tensor (kBar)[1]

6506.2126	756.4147	772.8926	-0.0000	0.0000	145.2842
756.4147	10526.6731	1590.2470	0.0000	-0.0000	-246.1990
772.8926	1590.2470	11108.2436	-0.0000	0.0000	680.1524
0.0000	0.0000	-0.0000	2022.0889	366.2653	0.0000
0.0000	-0.0000	0.0000	366.2653	5064.6324	-0.0000
145.2842	-246.1990	680.1524	0.0000	-0.0000	2293.3318

[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].