SACADA Database Code: 139

Topology: 3,4T86

# of independent nodes (IN): 2
Transitivity: [2563]
Space Group: P42/mmc
Pearson: tP24
Coordination Number (CN): 3, 4 (2:1)

Year: 2013

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
3,4T86 (SACADA #139)		2.301		0.887	236.3	123.2	15.6	SACADA[1]
3D (6,0)-II	35		Metal		231.08	131.00	43.0	doi: 10.1038/srep01331

Elasticity tensor (kBar)[1]

2837.8076	2327.6477	821.8776	0.0000	0.0000	0.0000
2327.6477	2837.8076	821.8776	-0.0000	-0.0000	0.0000
821.8776	821.8776	8592.1213	-0.0000	0.0000	0.0000
0.0000	-0.0000	-0.0000	1346.4137	0.0000	-0.0000
0.0000	0.0000	0.0000	0.0000	1742.7645	-0.0000
0.0000	0.0000	0.0000	-0.0000	-0.0000	1742.7643

[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].