SACADA Database Code: 205

Topology: 3^3,4T79

# of independent nodes (IN): 4
Transitivity: [4442]
Space Group: P42/mmc
Pearson: tP14
Coordination Number (CN): 3, 4 (6:1)

Year: 2013

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
3^3,4T79 (SACADA #205)		2.972		0.952	349.5	168.4	22.3	SACADA[1]
T14		2.923			349.6			doi: 10.1073/pnas.1311028110

Elasticity tensor (kBar)[1]

7416.1788	160.1285	1384.0453	0.0000	-0.0000	0.0000
160.1285	7416.1788	1384.0453	0.0000	0.0000	-0.0000
1384.0453	1384.0453	12097.7001	0.0000	-0.0000	-0.0000
0.0000	0.0000	0.0000	690.7002	0.0000	0.0000
-0.0000	0.0000	-0.0000	0.0000	972.1096	0.0000
0.0000	-0.0000	-0.0000	0.0000	0.0000	972.1081

[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].