SACADA Database Code: 184

Topology: 3^2,4T191

# of independent nodes (IN): 3
Transitivity: [3752]
Space Group: Cmcm
Pearson: oS24
Coordination Number (CN): 3, 4 (2:1)

Year: 2011

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
3^2,4T191 (SACADA #184)		2.952		0.805	292.4	199.3	23.0	SACADA[1]
3D-(7,0)		3.020			273.9	201.6	49.8	doi: 10.1021/nn202053t

Elasticity tensor (kBar)[1]

3168.6588	543.6014	142.8132	0.0000	-0.0000	-0.0000
543.6014	11740.0911	1698.6713	-0.0000	-0.0000	0.0000
142.8132	1698.6713	12161.8047	0.0000	-0.0000	0.0000
0.0000	-0.0000	0.0000	341.2941	0.0000	-0.0000
-0.0000	-0.0000	-0.0000	0.0000	4970.8980	0.0000
-0.0000	0.0000	0.0000	-0.0000	0.0000	1103.6660

[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].