SACADA Database Code: 223

Topology: 3^3,4T80

# of independent nodes (IN): 4
Transitivity: [4863]
Space Group: Immm
Pearson: oI28
Coordination Number (CN): 3, 4 (5:2)

Year: 2011

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
3^3,4T80 (SACADA #223)		2.868		0.788	171.4	141.1	20.8	SACADA[1]
3D-(8,0)		2.944			280.6	198.3	54.5	doi: 10.1021/nn202053t

Elasticity tensor (kBar)[1]

11450.6411	515.1814	1777.3853	0.0000	0.0000	0.0000
515.1814	2966.8560	-209.0174	0.0000	-0.0000	0.0000
1777.3853	-209.0174	12267.9993	0.0000	-0.0000	0.0000
0.0000	0.0000	0.0000	128.8264	-0.0000	0.0000
0.0000	-0.0000	-0.0000	-0.0000	810.4007	-0.0000
0.0000	0.0000	0.0000	0.0000	-0.0000	4973.1070

[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].