SACADA Database Code: 305

Topology: 4^9T3

# of independent nodes (IN): 9
Transitivity: [9(16)(12)3]
Space Group: Cmcm
Pearson: oS92
Coordination Number (CN): 4

Year: 2013

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^9T3 (SACADA #305)		3.045		0.767	359.4	401.2	75.1	SACADA[1]
KIX		3.01	3.56		357.2		82.4	doi: 10.1063/1.4802002

Elasticity tensor (kBar)[1]

9020.5292	918.1758	924.0567	0.0000	0.0000	-0.0000
918.1758	9092.7721	886.2784	-0.0000	-0.0000	-0.0000
924.0567	886.2784	8771.6960	-0.0000	-0.0000	0.0000
0.0000	-0.0000	-0.0000	3831.9846	-0.0000	0.0000
0.0000	-0.0000	-0.0000	0.0000	4178.7410	0.0000
-0.0000	0.0000	0.0000	0.0000	0.0000	4003.9088

[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].