SACADA Database Code: 80

Topology: dft

# of independent nodes (IN): 1
Transitivity: [1353]
Space Group: P42/mmc
Pearson: tP8
Coordination Number (CN): 4

Year: 2011

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
dft (SACADA #80)		2.919		0.642	340.0	253.5	32.0	SACADA[1]
TA3								doi: 10.1134/s1063776111060173
TA3								link

Elasticity tensor (kBar)[1]

9188.9597	581.4915	736.0166	0.0000	-0.0000	-0.0000
581.4915	9188.9597	736.0166	-0.0000	-0.0000	-0.0000
736.0166	736.0166	8151.8514	-0.0000	0.0000	0.0000
0.0000	0.0000	-0.0000	1310.3957	-0.0000	-0.0000
-0.0000	-0.0000	-0.0000	-0.0000	2183.9026	0.0000
-0.0000	0.0000	0.0000	-0.0000	0.0000	2183.9033

[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].