SACADA Database Code: 89

Topology: afi

# of independent nodes (IN): 1
Transitivity: [1464]
Space Group: P6/mcc
Pearson: hP24
Coordination Number (CN): 4

Year: 1993

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
24-hexa(2,0)afi (SACADA #89)		2.847		0.428	335.0	346.5	63.2	SACADA[1]
tubulane								doi: 10.1016/0009-2614(93)80059-X
TA7								doi: 10.1134/s1063776111060173
TA7								link
3D (6,0)-III			2.29		334.14	352.81	83.7	doi: 10.1038/srep01331

Elasticity tensor (kBar)[1]

7648.1205	1609.4867	196.2925	3.8157	1.1019	0.5101
1609.4867	7606.0898	200.6854	8.9536	6.5658	0.3266
196.2925	200.6854	11012.6860	17.7418	-2.3130	-0.5635
3.8157	8.9536	17.7418	3008.1509	7.5576	2.9083
1.1019	6.5658	-2.3130	7.5576	3288.6431	1.5398
0.5101	0.3266	-0.5635	2.9083	1.5398	3280.8408

[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].