SACADA Database Code: 88

Topology: ato

# of independent nodes (IN): 1
Transitivity: [1463]
Space Group: R-3m
Pearson: hR36
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
36-hexa(3,3)ato (SACADA #88)		3.045		0.542	355.0	331.5	56.7	SACADA[1]
tubulane								doi: 10.1016/0009-2614(93)80059-X
3D (3,3)-III					356.04	345.09	85.3	doi: 10.1038/srep01331
γ-C		1.56	2.43		341		72.4	doi: 10.1016/j.physleta.2015.06.037

Elasticity tensor (kBar)[1]

7548.5273	2209.6665	376.4896	0.0000	162.4227	0.0000
2209.6665	7548.5273	376.4896	0.0000	-162.4227	-0.0000
376.4896	376.4896	11008.9340	0.0000	-0.0000	-0.0000
0.0000	0.0000	0.0000	2669.4304	-0.0000	162.4227
162.4227	-162.4227	-0.0000	-0.0000	3331.1356	0.0000
0.0000	-0.0000	-0.0000	162.4227	0.0000	3331.1355

[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].