SACADA Database Code: 260

Topology: 4^6T16

# of independent nodes (IN): 6
Transitivity: [6996]
Space Group: Pmma
Pearson: oP20
Coordination Number (CN): 4

Year: 2015

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^6T16 (SACADA #260)		3.468		0.663	433.4	487.6	91.5	SACADA[1]
oP20	0-20	3.431	4.0		420		90.9	doi: 10.1039/c4cp04569f

Elasticity tensor (kBar)[1]

10540.2848	453.0912	1433.1860	-0.0000	-0.0000	-0.0000
453.0912	11886.3766	818.6447	0.0000	-0.0000	-0.0000
1433.1860	818.6447	11197.2462	0.0000	0.0000	-0.0000
-0.0000	0.0000	0.0000	4456.3969	0.0000	0.0000
-0.0000	-0.0000	0.0000	0.0000	4761.7001	0.0000
-0.0000	-0.0000	-0.0000	0.0000	0.0000	4929.4497

[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].