SACADA Database Code: 294

Topology: 4^8T15

# of independent nodes (IN): 8
Transitivity: [8(14)(13)7]
Space Group: P2/m
Pearson: mP16
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
4^8T15 (SACADA #294)		3.461		0.670	430.4	488.9	91.9	SACADA[1]
mP16	0-20	3.423	4.3		423		91.0	doi: 10.1039/c4cp04569f

Elasticity tensor (kBar)[1]

11581.5225	1035.5995	910.6955	-0.0000	0.0000	-39.4116
1035.5995	11600.4225	379.7056	0.0000	-0.0000	132.8269
910.6955	379.7056	10935.4250	0.0000	-0.0000	-150.7793
-0.0000	0.0000	0.0000	5383.9733	147.7013	-0.0000
0.0000	-0.0000	-0.0000	147.7013	4116.9929	-0.0000
-39.4116	132.8269	-150.7793	-0.0000	-0.0000	4496.1730

[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].