SACADA Database Code: 261

Topology: $3^2,4^4$T36

# of independent nodes (IN): 6
Transitivity: [6(10)73]
Space Group: I2/m
Pearson: mS24
Coordination Number (CN): 3, 4 (1:2)

Year: 2016

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
$3^2,4^4$T36 (SACADA #261)		3.200		0.255	294.4	319.2	59.3	SACADA[1]
mC24			0.06		329.0	356.3	65.3	doi: 10.1063/1.4952426

Elasticity tensor (kBar)[1]

10899.8037	1457.7147	1025.0592	0.0000	0.0000	933.8349
1457.7147	11948.9785	766.3271	0.0000	-0.0000	162.5952
1025.0592	766.3271	2803.0749	-0.0000	-0.0000	774.7371
0.0000	0.0000	-0.0000	5081.0730	614.3686	0.0000
0.0000	-0.0000	-0.0000	614.3686	2832.2704	0.0000
933.8349	162.5952	774.7371	0.0000	0.0000	2479.2397

[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].