SACADA Database Code: 191

Topology: $3,4^2T135$

# of independent nodes (IN): 3
Transitivity: [3883]
Space Group: Pmma
Pearson: oP20
Coordination Number (CN): 3, 4 (2:3)

Year: 2013

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
$3,4^2T135$ (SACADA #191)		2.637		0.977	285.7	206.9	25.1	SACADA[1]
3D (5,0)-II	35		0.82		284.21	220.27	84.5	doi: 10.1038/srep01331

Elasticity tensor (kBar)[1]

9204.9755	985.8228	651.6349	-0.0000	0.0000	-0.0000
985.8228	4634.0184	2747.6048	0.0000	0.0000	-0.0000
651.6349	2747.6048	3780.9398	0.0000	0.0000	0.0000
0.0000	-0.0000	0.0000	3188.1229	-0.0000	0.0000
0.0000	0.0000	-0.0000	0.0000	1967.9164	-0.0000
0.0000	-0.0000	0.0000	-0.0000	-0.0000	2506.1529

[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].