SACADA Database Code: 195

Topology: $3,4^2T243$

# of independent nodes (IN): 3
Transitivity: [3983]
Space Group: P4/mcc
Pearson: tP48
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
$3,4^2T243$ (SACADA #195)		2.488		0.378	290.8	163.2	19.7	SACADA[1]
4080-carbon		2.471	Semimetal		292	228	33	doi: 10.1063/1.4955055

Elasticity tensor (kBar)[1]

6229.4544	544.9661	1143.0032	0.0000	-0.0000	0.0000
544.9661	6229.4544	1143.0032	-0.0000	0.0000	0.0000
1143.0032	1143.0032	8479.2244	0.0000	0.0000	-0.0000
0.0000	-0.0000	-0.0000	264.1850	-0.0000	-0.0000
-0.0000	0.0000	0.0000	-0.0000	2617.9356	-0.0000
0.0000	0.0000	-0.0000	-0.0000	-0.0000	2617.9356

[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].