SACADA Database Code: 183

Topology: $3,4^2T209$

# of independent nodes (IN): 3
Transitivity: [3675]
Space Group: Cmmm
Pearson: oS20
Coordination Number (CN): 3, 4 (1:4)

Year: 2005

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
$3,4^2T209$ (SACADA #183)		3.364		0.763	403.7	414.5	75.4	SACADA[1]
(3,0)/(4,0)	17		Metal		397			doi: 10.1103/PhysRevB.72.214109
10B								doi: 10.1103/PhysRevB.88.014102
(3,0)/(4,0)			Metal					doi: 10.1063/1.4952426

Elasticity tensor (kBar)[1]

12049.1329	475.3179	1286.9114	-0.0000	0.0000	-0.0000
475.3179	12893.4723	371.7348	-0.0000	-0.0000	-0.0000
1286.9114	371.7348	7848.1625	-0.0000	-0.0000	0.0000
-0.0000	-0.0000	-0.0000	4945.8804	-0.0000	0.0000
0.0000	-0.0000	-0.0000	-0.0000	3316.5388	0.0000
-0.0000	-0.0000	0.0000	0.0000	0.0000	3006.2125

[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].