SACADA Database Code: 197

Topology: 3^2,4T202

# of independent nodes (IN): 3
Transitivity: -
Space Group: Pn-3m
Pearson: cP56
Coordination Number (CN): 3, 4 (6:1)

Year: 2009

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
3^2,4T202 (SACADA #197)		2.123		1.267	91.2	60.5	6.9	SACADA[1]
AHD C28 (2-fold)		2.18	1.31		122.8			doi: 10.1016/j.cplett.2009.03.033
		2.18			122.8			doi: 10.3103/s1063457610020012

Elasticity tensor (kBar)[1]

1433.4388	652.1615	652.1615	0.0000	-0.0000	0.0000
652.1615	1433.4388	652.1615	-0.0000	0.0000	-0.0000
652.1615	652.1615	1433.4388	-0.0000	0.0000	-0.0000
-0.0000	-0.0000	-0.0000	810.7447	0.0000	0.0000
-0.0000	0.0000	-0.0000	0.0000	810.7447	0.0000
0.0000	-0.0000	-0.0000	0.0000	0.0000	810.7447

[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].