SACADA Database Code: 136

Topology: 3,4T226

# of independent nodes (IN): 2
Transitivity: [2552]
Space Group: Cmcm
Pearson: oS24
Coordination Number (CN): 3, 4 (1:2)

Year: 2005

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
3,4T226 (SACADA #136)		3.213		0.309	369.7	376.8	68.3	SACADA[1]
(4,0)ab	40		2.3		361			doi: 10.1103/PhysRevB.72.214109
(4,0)ab			2.12		376.0	390.4	65.6	doi: 10.1063/1.4952426

Elasticity tensor (kBar)[1]

12408.9053	590.1588	324.1402	-0.0000	0.0000	0.0000
590.1588	9886.9631	2102.8148	-0.0000	0.0000	0.0000
324.1402	2102.8148	6024.5254	0.0000	-0.0000	0.0000
-0.0000	0.0000	0.0000	4813.4923	0.0000	-0.0000
0.0000	0.0000	-0.0000	0.0000	3301.9004	-0.0000
-0.0000	0.0000	0.0000	-0.0000	0.0000	3097.1946

[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].