

SACADA Database Code: 153

Topology: 4³T82

of independent nodes (IN): 3
Transitivity: [3332]
Space Group: I-4m2
Pearson: tI12
Coordination Number (CN): 4

Year: 2001

Data

Name	Pressure, GPa	Density, g/cm ³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4 ³ T82 (SACADA #153)		3.064		1.614	336.0	290.5	45.8	SACADA ¹
6(3)5-09		3.10						doi: 10.1016/S0009-2614(01)00126-9 17

Elasticity tensor (kBar)¹

6961.1367	1655.1333	1569.8497	-789.7809	1.6587	3.8313
1655.1333	7282.1551	803.8609	1014.1803	3.3393	-3.9178
1569.8497	803.8609	7958.2823	-465.3812	0.6049	3.8473
-789.7809	1014.1803	-465.3812	3058.9530	-1.8514	4.4988
1.6587	3.3393	0.6049	-1.8514	2279.4030	-625.6604
3.8313	-3.9178	3.8473	4.4988	-625.6604	3301.3604

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 $2\pi \times 0.025 \text{ \AA}^{-1}$ 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 $\text{\AA}^{-1}$ 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].