

SACADA Database Code: 227

Topology: 3⁴T15

of independent nodes (IN): 4
Transitivity: [4896]
Space Group: Pm-3m
Pearson: cP168
Coordination Number (CN): 3

Year: 2014

Data

Name	Pressure, GPa	Density, g/cm ³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
3 ⁴ T15 (SACADA #227)		1.116		0.828	87.4	36.8	5.2	SACADA ¹
8-4-2-P		1.16	0.38					doi: 10.1016/j.carbon.2014.04.077 

Elasticity tensor (kBar)¹

1363.7420	629.3012	629.3012	-0.0000	0.0000	-0.0000
629.3012	1363.7420	629.3012	-0.0000	0.0000	0.0000
629.3012	629.3012	1363.7420	0.0000	-0.0000	0.0000
-0.0000	-0.0000	0.0000	368.4245	-0.0000	-0.0000
0.0000	-0.0000	-0.0000	-0.0000	368.4245	-0.0000
-0.0000	0.0000	0.0000	-0.0000	0.0000	368.4245

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].