

SACADA Database Code: 360

Topology: 4⁷T21

of independent nodes (IN): 7
Transitivity: [7(16)(12)3]
Space Group: P-1
Pearson: aP14
Coordination Number (CN): 4

Year: 2017

Data

Name	Pressure, GPa	Density, g/cm ³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4 ⁷ T21 (SACADA #360)		3.476		0.872	404.8	461.2	86.8	SACADA ¹
G11								doi: 10.1002/cphc.201700151 ✉

Elasticity tensor (kBar)¹

11045.0955	795.9576	1096.1486	194.3591	-44.8639	-305.6759
795.9576	9638.6348	1557.9314	-183.3731	278.2791	213.3483
1096.1486	1557.9314	8904.0595	46.5300	-337.8841	-294.5845
194.3591	-183.3731	46.5300	5003.4066	-0.7939	139.3459
-44.8639	278.2791	-337.8841	-0.7939	4654.2929	266.9364
-305.6759	213.3483	-294.5845	139.3459	266.9364	4840.3085

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].