

SACADA Database Code: 382

Topology: 4⁶T32

of independent nodes (IN): 6
Transitivity: [6(12)(12)6]
Space Group: P21
Pearson: mP12
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 ⁶ T32 (SACADA #382)		3.521		0.819	416.0	484.5	91.5	SACADA ¹
G63								doi: 10.1002/cphc.201700151 ✉

Elasticity tensor (kBar)¹

10812.8742	742.4312	732.8747	0.0000	0.0000	-351.4072
742.4312	11809.5710	523.7317	0.0000	0.0000	167.7141
732.8747	523.7317	10839.3111	-0.0000	-0.0000	148.6126
0.0000	0.0000	-0.0000	5042.8788	284.9659	0.0000
0.0000	0.0000	-0.0000	284.9659	4648.0056	0.0000
-351.4072	167.7141	148.6126	0.0000	0.0000	4152.3959

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].