

SACADA Database Code: 434

Topology: 4⁸T38

of independent nodes (IN): 8
Transitivity: [8(16)(11)3]
Space Group: P21
Pearson: mP16
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 ⁸ T38 (SACADA #434)		3.399		0.891	389.5	434.4	81.3	SACADA ¹
G134								doi: 10.1002/cphc.201700151 ✉

Elasticity tensor (kBar)¹

10825.2619	1017.9376	727.4018	0.0000	0.0000	-146.1445
1017.9376	9092.5107	1416.6040	0.0000	0.0000	-32.8405
727.4018	1416.6040	8885.0317	-0.0000	-0.0000	128.7542
0.0000	0.0000	-0.0000	4751.0194	-323.2259	-0.0000
0.0000	0.0000	-0.0000	-323.2259	4469.3320	0.0000
-146.1445	-32.8405	128.7542	-0.0000	0.0000	4048.1352

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].