

SACADA Database Code: 611

Topology: 4³T188-CA

of independent nodes (IN): 3
Transitivity: [3885]
Space Group: Cmmm
Pearson: oS32
Coordination Number (CN): 4

Year: 2021

Data

Name	Pressure, GPa	Density, g/cm ³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4 ³ T188-CA (SACADA #611)		3.209		0.438	361.4	341.5	59.0	SACADA ¹
4 ³ T188-CA								doi: 10.1038/s41524-021-00491-y ↗

Elasticity tensor (kBar)¹

9899.0763	1019.4250	1392.8523	0.0000	0.0000	0.0000
1019.4250	6497.4496	1006.0313	0.0000	-0.0000	0.0000
1392.8523	1006.0313	10015.4456	0.0000	-0.0000	-0.0000
0.0000	0.0000	0.0000	2984.1859	-0.0000	-0.0000
0.0000	-0.0000	-0.0000	-0.0000	2620.2632	0.0000
0.0000	-0.0000	-0.0000	-0.0000	0.0000	4192.3212

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].