

SACADA Database Code: 405

Topology: 4³T174

of independent nodes (IN): 3
Transitivity: [3452]
Space Group: I-42d
Pearson: tI28
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 ³ T174 (SACADA #405)		3.405		0.981	383.5	427.5	80.0	SACADA ¹
G96								doi: 10.1002/cphc.201700151 d

Elasticity tensor (kBar)¹

8666.7216	1127.5436	1247.0022	0.0000	-0.0000	-0.0000
1127.5436	8666.7216	1247.0022	-0.0000	0.0000	-0.0000
1247.0022	1247.0022	10024.8875	-0.0000	-0.0000	-0.0000
0.0000	-0.0000	-0.0000	4229.1720	-0.0000	0.0000
-0.0000	0.0000	-0.0000	-0.0000	4654.0201	0.0000
-0.0000	-0.0000	-0.0000	-0.0000	0.0000	4654.0201

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].