

SACADA Database Code: 244

Topology: 4⁵T12

of independent nodes (IN): 5
Transitivity: [5894]
Space Group: C2/c
Pearson: mS32
Coordination Number (CN): 4

Year: 2012

Data

Name	Pressure, GPa	Density, g/cm ³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4 ⁵ T12 (SACADA #244)		3.387		0.755	416.2	462.2	86.4	SACADA ¹
X-carbon								doi: 10.1103/PhysRevB.85.201407 
X-carbon								doi: 10.1021/ja304380p 
X-carbon								doi: 10.3103/s1063457612060093 
X-carbon					404			doi: 10.1016/j.carbon.2014.06.050 
X-carbon								doi: 10.1088/0256-307x/32/9/096201 

Elasticity tensor (kBar)¹

9595.0698	1217.3194	1151.9173	0.0000	-0.0000	839.1831
1217.3194	10822.1833	1235.5673	0.0000	0.0000	106.2874
1151.9173	1235.5673	9886.3234	-0.0000	-0.0000	-487.0821
0.0000	0.0000	-0.0000	4958.5173	338.9060	-0.0000
-0.0000	0.0000	0.0000	338.9060	4693.6637	-0.0000
839.1831	106.2874	-487.0821	-0.0000	-0.0000	4590.3126

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 [\[9\]](#).