SACADA Database Code: 429

Topology: 4^{16}T11

# of independent nodes (IN): 16
Transitivity: [(16)(32)(25)9]
Space Group: P1
Pearson: aP16
Coordination Number (CN): 4

Year: 2017

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^{16}T11 (SACADA #429)		3.399		0.956	390.6	429.2	80.0	SACADA[1]
G129								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

9896.1645	1086.7397	1008.8042	-130.5249	-193.6564	7.1562
1086.7397	9549.8944	1067.4125	714.9478	57.2058	22.6224
1008.8042	1067.4125	9420.6068	-183.9736	-338.0673	358.7045
-130.5249	714.9478	-183.9736	4288.5484	100.3716	-68.4858
-193.6564	57.2058	-338.0673	100.3716	4121.6451	-18.7034
7.1562	22.6224	358.7045	-68.4858	-18.7034	4504.7017

[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 $2\pi \times 0.025$ Å^{-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 Å^{-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].