SACADA Database Code: 455

Topology: 4^{16}T15

# of independent nodes (IN): 16
Transitivity: [(16)(32)(26)(10)]
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}T15 (SACADA #455)		3.409		0.852	397.5	443.5	83.0	SACADA[1]
G162								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

9125.9510	1336.3992	1460.3330	132.6868	3.1964	-36.6533
1336.3992	9855.5315	1162.7606	68.9873	-63.8722	-93.2249
1460.3330	1162.7606	8889.9861	-16.8634	-14.4290	105.7209
132.6868	68.9873	-16.8634	4812.6448	-179.9985	103.3424
3.1964	-63.8722	-14.4290	-179.9985	4577.8275	-52.2157
-36.6533	-93.2249	105.7209	103.3424	-52.2157	4922.3975

[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].