SACADA Database Code: 469

Topology: 4^{16}T22

# of independent nodes (IN): 16
Transitivity: [(16)(32)(23)7]
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}T22 (SACADA #469)		3.339		0.843	390.5	419.3	77.6	SACADA[1]
G177								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

9204.2926	1115.1374	907.4248	-490.4176	4.7245	134.5866
1115.1374	9331.4174	1493.7950	-85.3223	-332.2056	-14.1009
907.4248	1493.7950	9605.5081	-97.7237	35.9420	145.9004
-490.4176	-85.3223	-97.7237	4090.1757	-49.9166	-123.0427
4.7245	-332.2056	35.9420	-49.9166	4630.6527	-163.7467
134.5866	-14.1009	145.9004	-123.0427	-163.7467	4083.6243

[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].