SACADA Database Code: 449

Topology: 4^{14}T3

# of independent nodes (IN): 14
Transitivity: [(14)(28)(17)3]
Space Group: P1
Pearson: aP14
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^{14}T3 (SACADA #449)		3.427		0.881	403.1	446.6	83.5	SACADA[1]
G156								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

8681.4217	1274.0736	1477.2427	-257.2506	48.4369	238.9661
1274.0736	10210.6797	1035.4502	27.2312	-143.7965	67.0767
1477.2427	1035.4502	9866.4105	127.6345	-151.9431	-120.7503
-257.2506	27.2312	127.6345	4640.6731	141.6041	-241.4435
48.4369	-143.7965	-151.9431	141.6041	4635.3387	18.3846
238.9661	67.0767	-120.7503	-241.4435	18.3846	4830.2554

[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].