SACADA Database Code: 501

Topology: 4^{14}T4

# of independent nodes (IN): 14
Transitivity: [(14)(28)(18)4]
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}T4 (SACADA #501)		3.286		1.068	373.4	369.4	65.9	SACADA[1]
G214								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

8538.0071	1115.5881	1553.1185	-407.5732	-17.7898	161.5729
1115.5881	9216.4546	937.6951	206.6711	309.1271	59.2054
1553.1185	937.6951	8639.8948	24.3113	-146.9942	394.6897
-407.5732	206.6711	24.3113	3543.7153	175.8704	115.6329
-17.7898	309.1271	-146.9942	175.8704	3870.2498	-171.6925
161.5729	59.2054	394.6897	115.6329	-171.6925	3508.0758

[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].