SACADA Database Code: 503

Topology: 4^{14}T5

# of independent nodes (IN): 14
Transitivity: [(14)(28)(29)(15)]
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}T5 (SACADA #503)		3.448		1.026	381.9	433.6	81.5	SACADA[1]
G216								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

11330.1982	556.5527	513.6441	-95.1452	42.2085	-110.5511
556.5527	9106.9358	1388.2568	-159.7456	-584.8830	-177.2061
513.6441	1388.2568	9079.4177	144.9367	518.2400	185.7624
-95.1452	-159.7456	144.9367	4472.1796	43.0320	-80.3958
42.2085	-584.8830	518.2400	43.0320	4081.7667	144.7171
-110.5511	-177.2061	185.7624	-80.3958	144.7171	4317.3044

[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].