SACADA Database Code: 464

Topology: 4^{16}T21

# of independent nodes (IN): 16
Transitivity: [(16)(32)(21)5]
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}T21 (SACADA #464)		3.287		0.954	376.8	377.9	68.0	SACADA[1]
G172								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

8468.0922	1353.1581	1343.6932	177.8509	85.6694	129.4373
1353.1581	8804.5685	1132.7204	304.0445	158.5912	30.2540
1343.6932	1132.7204	8980.8025	245.7557	-184.3665	124.8645
177.8509	304.0445	245.7557	3655.9666	-89.6264	314.1369
85.6694	158.5912	-184.3665	-89.6264	3958.3366	92.4366
129.4373	30.2540	124.8645	314.1369	92.4366	3854.4834

[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].