SACADA Database Code: 424

Topology: 4^8T33

# of independent nodes (IN): 8
Transitivity: [8(19)(12)3]
Space Group: P-1
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
4^8T33 (SACADA #424)		3.411		0.963	384.8	440.5	82.9	SACADA[1]
G124								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

9147.8381	1258.5202	1049.7790	-419.1390	-115.4534	-488.7982
1258.5202	9709.9718	602.7033	-584.6571	-183.3269	-4.1902
1049.7790	602.7033	9953.3618	173.0811	531.8542	-282.8831
-419.1390	-584.6571	173.0811	4516.3334	-191.9367	41.1391
-115.4534	-183.3269	531.8542	-191.9367	4164.3975	79.2383
-488.7982	-4.1902	-282.8831	41.1391	79.2383	4796.5585

[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].