SACADA Database Code: 432

Topology: 4^8T37

# of independent nodes (IN): 8
Transitivity: [8(18)(11)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
4^8T37 (SACADA #432)		3.276		0.938	375.2	384.2	69.8	SACADA[1]
G132								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

9595.8659	1374.3779	800.5212	48.6002	-148.1567	540.7812
1374.3779	8592.4950	1022.0806	-91.3449	19.7861	-290.7739
800.5212	1022.0806	9210.9166	-5.4593	141.7540	587.4403
48.6002	-91.3449	-5.4593	3944.2181	309.7707	-79.7958
-148.1567	19.7861	141.7540	309.7707	3902.3764	19.1444
540.7812	-290.7739	587.4403	-79.7958	19.1444	3366.5936

[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].