SACADA Database Code: 511

Topology: 4^8T49

# of independent nodes (IN): 8
Transitivity: [8(14)(12)7]
Space Group: I2/m
Pearson: mS32
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
4^8T49 (SACADA #511)		3.461		0.664	412.9	475.9	89.7	SACADA[1]
G225								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

10010.9135	701.6301	989.4691	-0.0000	-0.0000	275.4464
701.6301	11029.2409	759.2957	-0.0000	-0.0000	-436.5501
989.4691	759.2957	11263.1793	0.0000	0.0000	13.6190
-0.0000	-0.0000	0.0000	4362.7423	-500.6916	0.0000
-0.0000	-0.0000	0.0000	-500.6916	4967.3011	-0.0000
275.4464	-436.5501	13.6190	0.0000	-0.0000	4566.0522

[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].