SACADA Database Code: 426

Topology: 4^8T34

# of independent nodes (IN): 8
Transitivity: [8(17)(13)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
4^8T34 (SACADA #426)		3.456		0.987	390.0	445.2	83.8	SACADA[1]
G126								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

10572.1749	967.5625	793.0656	522.3740	-284.2647	323.7669
967.5625	10245.2232	584.1970	171.0409	-66.2137	159.9828
793.0656	584.1970	9636.9040	-313.7597	416.1110	87.0493
522.3740	171.0409	-313.7597	4617.6022	271.3805	-84.8130
-284.2647	-66.2137	416.1110	271.3805	4089.4036	-196.4292
323.7669	159.9828	87.0493	-84.8130	-196.4292	4259.0459

[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].