SACADA Database Code: 470

Topology: 4^8T44

# of independent nodes (IN): 8
Transitivity: [8(16)(16)8]
Space Group: P21
Pearson: mP16
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
4^8T44 (SACADA #470)		3.531		0.750	421.3	495.0	93.6	SACADA[1]
G178								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

10979.9639	819.7204	634.3955	-0.0000	0.0000	-343.9098
819.7204	11803.6532	564.0248	-0.0000	-0.0000	261.9239
634.3955	564.0248	11118.1589	0.0000	0.0000	118.1255
-0.0000	-0.0000	0.0000	5129.4854	362.3714	-0.0000
-0.0000	-0.0000	0.0000	362.3714	4761.1440	-0.0000
-343.9098	261.9239	118.1255	0.0000	-0.0000	4313.2857

[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].