SACADA Database Code: 445

Topology: 4^6T37

# of independent nodes (IN): 6
Transitivity: [6(14)92]
Space Group: P-1
Pearson: aP12
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
4^6T37 (SACADA #445)		3.376		0.798	398.9	437.2	81.5	SACADA[1]
G151								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

8793.7065	1742.5103	1032.4160	100.6696	156.6752	43.7150
1742.5103	8827.5202	1020.2716	-65.8487	-193.0896	81.0835
1032.4160	1020.2716	10747.7832	146.6321	-296.9686	-235.4079
100.6696	-65.8487	146.6321	4626.4330	-143.7489	-38.5901
156.6752	-193.0896	-296.9686	-143.7489	4570.2370	376.5069
43.7150	81.0835	-235.4079	-38.5901	376.5069	4623.2875

[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].