SACADA Database Code: 509

Topology: 4^5T61

# of independent nodes (IN): 5
Transitivity: [5(12)82]
Space Group: P-1
Pearson: aP10
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
4^5T61 (SACADA #509)		3.219		1.129	350.0	349.8	62.8	SACADA[1]
G222								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

7569.1768	1035.2847	1248.2690	-73.9117	-62.2955	256.7864
1035.2847	9521.6229	881.0903	-399.1539	272.8187	166.8399
1248.2690	881.0903	8181.8351	-249.3412	100.1166	-40.0371
-73.9117	-399.1539	-249.3412	3267.8044	-72.9002	-20.5600
-62.2955	272.8187	100.1166	-72.9002	3228.1137	103.8801
256.7864	166.8399	-40.0371	-20.5600	103.8801	3713.9693

[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].