SACADA Database Code: 376

Topology: 4^6T31

# of independent nodes (IN): 6
Transitivity: [6(13)(10)1]
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
4^6T31 (SACADA #376)		3.239		1.022	363.1	370.0	67.0	SACADA[1]
G52								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

7823.2695	1622.7193	1281.4678	294.4292	-34.8685	-196.9841
1622.7193	9305.2540	1044.6870	52.7828	-100.1623	-31.8494
1281.4678	1044.6870	7781.8000	-35.7337	265.6230	91.0264
294.4292	52.7828	-35.7337	4172.3652	-34.5481	-86.2578
-34.8685	-100.1623	265.6230	-34.5481	3619.4504	-414.6806
-196.9841	-31.8494	91.0264	-86.2578	-414.6806	3813.8607

[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].