SACADA Database Code: 522

Topology: 4^6T50

# of independent nodes (IN): 6
Transitivity: [6(13)(13)4]
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
4^6T50 (SACADA #522)		3.361		1.446	172.6	174.6	31.5	SACADA[1]
G245								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

10144.5401	1394.6613	-6.5536	-171.2595	-150.3062	184.3391
1394.6613	7897.4924	1505.6852	-65.1080	-504.0364	-246.4276
-6.5536	1505.6852	7230.3741	-237.5452	-507.8756	-512.9529
-171.2595	-65.1080	-237.5452	3967.7131	-206.0755	-684.7697
-150.3062	-504.0364	-507.8756	-206.0755	3279.9950	-217.4583
184.3391	-246.4276	-512.9529	-684.7697	-217.4583	2751.1646

[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].