SACADA Database Code: 521

Topology: 4^6T49

# of independent nodes (IN): 6
Transitivity: [6(13)(10)3]
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
4^6T49 (SACADA #521)		3.271		1.180	345.1	349.6	63.2	SACADA[1]
G244								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

9520.2891	1234.8088	600.3980	-34.1123	-28.9565	-124.2452
1234.8088	7609.2128	1169.9452	-28.0174	19.0294	467.4718
600.3980	1169.9452	8025.9322	-142.7319	-308.7966	-418.6149
-34.1123	-28.0174	-142.7319	3702.0535	384.7874	-149.9443
-28.9565	19.0294	-308.7966	384.7874	3267.3252	-80.2964
-124.2452	467.4718	-418.6149	-149.9443	-80.2964	3239.1818

[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].