SACADA Database Code: 500

Topology: 4^7T30

# of independent nodes (IN): 7
Transitivity: [7(11)(11)6]
Space Group: P21/m
Pearson: mP14
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
4^7T30 (SACADA #500)		3.439		0.731	405.9	452.5	84.7	SACADA[1]
G213								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

10898.0142	978.7320	839.3035	0.0000	-0.0000	195.2089
978.7320	10785.1908	502.1382	0.0000	-0.0000	-206.4975
839.3035	502.1382	10238.3722	0.0000	0.0000	20.6480
0.0000	0.0000	0.0000	5061.5137	-287.2000	-0.0000
-0.0000	-0.0000	0.0000	-287.2000	3947.4130	0.0000
195.2089	-206.4975	20.6480	-0.0000	0.0000	3909.2741

[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].