SACADA Database Code: 361

Topology: 4^7T22

# of independent nodes (IN): 7
Transitivity: [7(12)(10)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
4^7T22 (SACADA #361)		3.419		0.674	409.2	466.1	87.7	SACADA[1]
G12								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

10238.2592	896.3909	855.9844	0.0000	0.0000	-214.1573
896.3909	10987.8706	487.5045	0.0000	0.0000	318.6949
855.9844	487.5045	11131.1236	-0.0000	-0.0000	-182.6344
0.0000	0.0000	-0.0000	4853.5595	408.1483	0.0000
0.0000	0.0000	-0.0000	408.1483	4540.8090	-0.0000
-214.1573	318.6949	-182.6344	0.0000	-0.0000	3978.3081

[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].