SACADA Database Code: 399

Topology: 4^5T53

# of independent nodes (IN): 5
Transitivity: [5(10)95]
Space Group: I2/a
Pearson: mS32
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
4^5T53 (SACADA #399)		3.488		0.861	408.0	471.9	89.0	SACADA[1]
G90								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

10163.9451	1731.9271	580.4327	-0.0001	0.0000	-636.7958
1731.9271	9125.0166	726.8601	-0.0001	0.0000	197.7206
580.4327	726.8601	11394.5310	-0.0000	0.0000	-582.9563
-0.0001	-0.0001	-0.0000	5189.7487	-220.9364	0.0000
0.0000	0.0000	0.0000	-220.9364	4585.4910	-0.0000
-636.7958	197.7206	-582.9563	0.0000	-0.0000	4744.2082

[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].