SACADA Database Code: 304

Topology: 4^9T5

# of independent nodes (IN): 9
Transitivity: [9(15)(14)8]
Space Group: C2/m
Pearson: mS36
Coordination Number (CN): 4

Year: 2013

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^9T5 (SACADA #304)		3.447		0.649	414.5	476.1	89.7	SACADA[1]
18A	20							doi: 10.1103/PhysRevB.88.014102

Elasticity tensor (kBar)[1]

11239.5396	557.8872	797.8256	-0.0000	0.0000	262.1240
557.8872	11076.8999	879.1747	-0.0000	0.0000	-369.7081
797.8256	879.1747	10514.9278	-0.0000	0.0000	123.5112
-0.0000	-0.0000	-0.0000	4682.7465	-456.0835	0.0000
0.0000	0.0000	0.0000	-456.0835	4877.8127	-0.0000
262.1240	-369.7081	123.5112	0.0000	-0.0000	4126.5191

[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].