SACADA Database Code: 302

Topology: 4^9T4

# of independent nodes (IN): 9
Transitivity: [9(14)(14)8]
Space Group: P21/m
Pearson: mP18
Coordination Number (CN): 4

Year: 2014

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^9T4 (SACADA #302)		3.448		0.647	414.9	476.5	89.8	SACADA[1]
M585		3.507	4.212		462.3		78.85	doi: 10.1016/j.ssc.2013.11.035
M585								doi: 10.1088/0256-307x/32/9/096201
M585								doi: 10.1103/PhysRevB.93.085201

Elasticity tensor (kBar)[1]

11179.2211	440.9583	943.6020	0.0000	0.0000	-282.1277
440.9583	11072.7737	1015.1692	-0.0000	0.0000	-260.5211
943.6020	1015.1692	10286.4476	-0.0000	-0.0000	411.6091
0.0000	-0.0000	-0.0000	4495.7117	-386.2582	0.0000
0.0000	0.0000	-0.0000	-386.2582	5086.5148	-0.0000
-282.1277	-260.5211	411.6091	0.0000	-0.0000	4270.5947

[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].