SACADA Database Code: 214

Topology: 4^4T75

# of independent nodes (IN): 4
Transitivity: [4664]
Space Group: P2221
Pearson: oP10
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
4^4T75 (SACADA #214)		3.348		0.780	414.3	440.2	81.2	SACADA[1]
iceVI-carbon		3.30	3.59		396.4			doi: 10.1021/jp5080048

Elasticity tensor (kBar)[1]

10852.2833	1339.0353	1075.8496	0.0000	0.0000	0.0000
1339.0353	9325.7695	1694.7649	0.0000	0.0000	-0.0000
1075.8496	1694.7649	8955.8817	0.0000	-0.0000	-0.0000
0.0000	-0.0000	0.0000	3786.7166	-0.0000	0.0000
0.0000	-0.0000	-0.0000	-0.0000	4906.7922	0.0000
0.0000	-0.0000	-0.0000	0.0000	0.0000	5182.8906

[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].