SACADA Database Code: 283

Topology: 4^7T11

# of independent nodes (IN): 7
Transitivity: [7(14)(11)3]
Space Group: P21/c
Pearson: mP28
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
4^7T11 (SACADA #283)		3.200		1.261	352.4	316.1	52.0	SACADA[1]
iceV-carbon		3.15	3.78		333.8			doi: 10.1021/jp5080048

Elasticity tensor (kBar)[1]

7138.3332	1071.8469	1652.5428	-0.0000	0.0000	-183.6733
1071.8469	7161.0163	1861.9077	0.0000	-0.0000	-59.2530
1652.5428	1861.9077	8467.5428	-0.0000	0.0000	559.4072
-0.0000	-0.0000	-0.0000	2983.3283	176.5755	0.0000
0.0000	-0.0000	-0.0000	176.5755	3641.6068	-0.0000
-183.6733	-59.2530	559.4072	0.0000	0.0000	3186.7812

[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].