SACADA Database Code: 341

Topology: ajk5

# of independent nodes (IN): 17
Transitivity: [(17)(28)(26)(18)]
Space Group: P6/mmm
Pearson: hP200
Coordination Number (CN): 4

Year: 2011

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
ajk5 (SACADA #341)		3.311		0.786	378.3	438.8	82.8	SACADA[1]
clathrates IV-100		3.30			419			doi: 10.1021/jp205676p
clathrates IV-100		3.30	6.8					doi: 10.1021/ic102178d

Elasticity tensor (kBar)[1]

9591.4913	879.5238	851.4676	-0.0000	0.0000	0.0000
879.5238	9591.4913	851.4676	-0.0000	-0.0000	0.0000
851.4676	851.4676	9702.2732	-0.0000	0.0000	0.0000
-0.0000	-0.0000	-0.0000	4355.9837	-0.0000	0.0000
0.0000	-0.0000	0.0000	-0.0000	4409.2400	-0.0000
-0.0000	-0.0000	0.0000	0.0000	-0.0000	4409.2400

[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].