SACADA Database Code: 342

Topology: sig

# of independent nodes (IN): 17
Transitivity: [(17)(29)(20)5]
Space Group: P42/mnm
Pearson: tP172
Coordination Number (CN): 4

Year: 1998

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
sig (SACADA #342)		3.077		0.705	366.0	417.9	78.6	SACADA[1]
clathrates III								link
clathrates III		3.07			400			doi: 10.1021/jp205676p
clathrates III		3.07	6.1					doi: 10.1021/ic102178d

Elasticity tensor (kBar)[1]

9127.9235	943.6236	968.9382	-0.0000	-0.0000	0.0000
943.6236	9127.9235	968.9382	0.0000	0.0000	-0.0000
968.9382	968.9382	8926.1561	0.0000	-0.0000	-0.0000
-0.0000	0.0000	-0.0000	4191.4314	-0.0000	0.0000
-0.0000	0.0000	-0.0000	0.0000	4305.4284	0.0000
-0.0000	0.0000	-0.0000	0.0000	0.0000	4305.4284

[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].