SACADA Database Code: 220

Topology: doh

# of independent nodes (IN): 4
Transitivity: [4763]
Space Group: P6/mmm
Pearson: hP34
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
doh (SACADA #220)		3.003		0.731	372.1	390.6	71.7	SACADA[1]
clathrate H		3.00	5.6					doi: 10.1021/ic102178d

Elasticity tensor (kBar)[1]

9072.1606	964.3340	1169.0144	-0.0000	-0.0000	0.0000
964.3340	9072.1606	1169.0144	-0.0000	0.0000	-0.0000
1169.0144	1169.0144	8737.5775	0.0000	-0.0000	0.0000
-0.0000	0.0000	-0.0000	4053.9133	-0.0000	0.0000
0.0000	0.0000	-0.0000	-0.0000	3812.6985	0.0000
0.0000	-0.0000	0.0000	0.0000	0.0000	3812.6985

[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].