## SACADA Database Code: 300

Topology: ajk2

# of independent nodes (IN): 9
Transitivity: [9(13)(11)9]
Space Group: Fd-3m
Pearson: cF680
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
ajk2 (SACADA #300)		3.346		0.189				SACADA <sup>1</sup>
clathrates II-100		3.30			427			doi: 10.1021/jp205676p
clathrates II-100		3.30	6.9					doi: 10.1021/ic102178d ದ

<sup>1</sup> 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  $\Gamma$ -centered k-points mesh with a reciprocal-space resolution of  $2\pi \times 0.025$  Å<sup>-1</sup> is applied. We used tetrahedron method with Blöchl corrections to perform the k-point integration. The convergence thresholds are set at 10<sup>-6</sup> eV for energy and 10<sup>-5</sup> eV Å<sup>-1</sup> for ionic forces. Polycrystalline elastic moduli — the bulk modulus, the shear modulus, Young's modulus, and the Poisson's ratio  $\nu$  — have been calculated within the Voigt-Reuss-Hill [8] approximation. The Vicker's hardness H<sub>v</sub> has been estimated according to Oganov's model [9].