

SACADA Database Code: 163

Topology: alb-x-d

of independent nodes (IN): 3
Transitivity: [3442]
Space Group: P6/mmm
Pearson: hP16
Coordination Number (CN): 4

Year: 2013

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
alb-x-d (SACADA #163)		2.812		0.940	325.4	319.9	56.8	SACADA ¹
hex-C16								doi: 10.1007/978-94-007-6371-5_4

Elasticity tensor (kBar)¹

8449.7885	842.9353	761.4639	0.0000	0.0000	0.0000
842.9353	8449.7885	761.4639	0.0000	-0.0000	-0.0000
761.4639	761.4639	7687.6022	0.0000	0.0000	-0.0000
0.0000	0.0000	0.0000	3803.4266	0.0000	-0.0000
0.0000	-0.0000	0.0000	0.0000	2536.8153	0.0000
0.0000	-0.0000	-0.0000	-0.0000	0.0000	2536.8152

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 $2\pi \times 0.025 \text{ \AA}^{-1}$ 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 $\text{\AA}^{-1}$ 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].