SACADA Database Code: 94

Topology: dmd

# of independent nodes (IN): 2
Transitivity: [2232]
Space Group: P42/mmc
Pearson: tP6
Coordination Number (CN): 3, 4 (2:1)

Year: 2013

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
dmd (SACADA #94)		2.297		0.660	260.9	82.9	12.6	SACADA[1]
Exocyclo-butadieneite		2.27	0.5					doi: 10.1007/s10910-012-0115-6

Elasticity tensor (kBar)[1]

5994.7936	279.7160	952.6697	0.0000	0.0000	-0.0000
279.7160	5994.7936	952.6697	0.0000	-0.0000	0.0000
952.6697	952.6697	7362.5612	-0.0000	0.0000	-0.0000
0.0000	0.0000	-0.0000	66.7854	0.0000	0.0000
0.0000	-0.0000	0.0000	0.0000	594.3927	0.0000
-0.0000	0.0000	-0.0000	0.0000	0.0000	594.3927

[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].