SACADA Database Code: 105

Topology: jeb

# of independent nodes (IN): 2
Transitivity: [2332]
Space Group: Cmmm
Pearson: oS8
Coordination Number (CN): 3, 4 (1:1)

Year: 2012

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
jeb (SACADA #105)		3.074		0.904	334.9	200.9	23.3	SACADA[1]
isoglitter		3.009						doi: 10.1007/s10910-012-0030-x

Elasticity tensor (kBar)[1]

4836.0412	275.6034	642.2201	0.0000	0.0000	0.0000
275.6034	11688.1608	1769.8239	0.0000	-0.0000	-0.0000
642.2201	1769.8239	11226.1288	0.0000	-0.0000	0.0000
0.0000	0.0000	0.0000	1146.1682	0.0000	0.0000
0.0000	-0.0000	-0.0000	0.0000	5052.7249	-0.0000
0.0000	-0.0000	0.0000	0.0000	-0.0000	315.6251

[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].