SACADA Database Code: 119

Topology: mjb

# of independent nodes (IN): 2
Transitivity: [2343]
Space Group: P4/mmm
Pearson: tP8
Coordination Number (CN): 3, 4 (1:1)

Year: 2011

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
mjb (SACADA #119)		2.349		0.848	275.0	127.2	17.2	SACADA[1]
3D-(4,4)		2.344			277.6	140.4	79.8	doi: 10.1021/nn202053t
Squaroglitter		2.32	1.0		260			doi: 10.1021/ct4004367

Elasticity tensor (kBar)[1]

5745.9053	924.6154	665.8784	0.0000	-0.0000	-0.0000
924.6154	5745.9053	665.8784	-0.0000	-0.0000	0.0000
665.8784	665.8784	9202.2666	0.0000	0.0000	-0.0000
0.0000	-0.0000	0.0000	90.9209	-0.0000	-0.0000
-0.0000	-0.0000	0.0000	-0.0000	2245.6113	0.0000
-0.0000	0.0000	-0.0000	-0.0000	0.0000	2245.6113

[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].