SACADA Database Code: 130

Topology: fsg-3,4-Cmmm-2

# of independent nodes (IN): 2
Transitivity: [2453]
Space Group: Cmmm
Pearson: oS16
Coordination Number (CN): 3, 4 (1:1)

Year: 1999

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
fsg-3,4-Cmmm-2 (SACADA #130)		2.795		0.991	294.9	237.3	33.7	SACADA[1]
diamcr43bo		2.673						doi: 10.1006/jssc.1999.8448

Elasticity tensor (kBar)[1]

8274.9217	1511.6189	1329.1766	-0.0000	-0.0000	0.0000
1511.6189	3494.9837	922.7936	-0.0000	-0.0000	-0.0000
1329.1766	922.7936	9800.6500	0.0000	0.0000	-0.0000
-0.0000	-0.0000	0.0000	1767.5523	0.0000	0.0000
-0.0000	0.0000	0.0000	0.0000	1439.8352	-0.0000
0.0000	-0.0000	-0.0000	0.0000	-0.0000	4022.5482

[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].