SACADA Database Code: 109

Topology: fsd-3,4-I4/mcm

# of independent nodes (IN): 2
Transitivity: [2332]
Space Group: I4/mcm
Pearson: tI24
Coordination Number (CN): 3, 4 (1:2)

Year: 2015

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
fsd-3,4-I4/mcm (SACADA #109)		2.606		0.746	299.0	216.7	26.4	SACADA[1]
bct-C12			Metal		315.9	225.4	31.6	doi: 10.1038/srep10713

Elasticity tensor (kBar)[1]

5645.3392	1030.6562	801.9977	-2.6530	0.7496	0.1767
1030.6562	5668.0092	809.2401	5.0966	-1.7676	0.2256
801.9977	809.2401	11514.3360	5.0597	1.0276	-0.5143
-2.6530	5.0966	5.0597	663.2044	-1.4429	0.2596
0.7496	-1.7676	1.0276	-1.4429	2825.0560	0.2523
0.1767	0.2256	-0.5143	0.2596	0.2523	2824.7160

[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].