SACADA Database Code: 451

Topology: mbc-4,4-Imma

# of independent nodes (IN): 2
Transitivity: [2552]
Space Group: Imma
Pearson: oI16
Coordination Number (CN): 4

Year: 2017

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
mbc-4,4-Imma (SACADA #451)		3.307		0.853	383.9	398.2	72.8	SACADA[1]
G158								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

9367.8759	552.9831	2022.4297	0.0000	0.0000	-149.1500
552.9831	10569.3096	623.6750	-0.0000	0.0000	-18.8881
2022.4297	623.6750	8257.4487	-0.0000	0.0000	617.0891
0.0000	-0.0000	-0.0000	3926.8773	-172.0680	0.0000
0.0000	0.0000	0.0000	-172.0680	4328.5027	-0.0000
-149.1500	-18.8881	617.0891	0.0000	-0.0000	3521.3944

[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].