SACADA Database Code: 147

Topology: 4^2T112

# of independent nodes (IN): 2
Transitivity: -
Space Group: A2/n
Pearson: mS12
Coordination Number (CN): 4

Year: 2011

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^2T112 (SACADA #147)		3.475		0.900	428.9	481.5	90.3	SACADA[1]
mC12			2.82		399.5		84.4	doi: 10.1103/PhysRevB.84.161411
mC12								doi: 10.1038/srep00471

Elasticity tensor (kBar)[1]

10190.3106	1919.1333	1082.7688	0.0000	-0.0000	-571.8328
1919.1333	8898.9747	561.4576	-0.0000	0.0000	-85.9771
1082.7688	561.4576	12608.1996	-0.0000	0.0000	-68.2119
0.0000	-0.0000	-0.0000	4822.0972	-308.3955	-0.0000
-0.0000	-0.0000	0.0000	-308.3955	4490.0949	0.0000
-571.8328	-85.9771	-68.2119	-0.0000	0.0000	5669.7140

[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].