SACADA Database Code: 291

Topology: 4^8T16

# of independent nodes (IN): 8
Transitivity: [8(14)(12)7]
Space Group: C2/m
Pearson: mS32
Coordination Number (CN): 4

Year: 2015

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^8T16 (SACADA #291)		3.456		0.675	429.1	490.0	92.2	SACADA[1]
mS32	0-20	3.418	4.5		415		90.8	doi: 10.1039/c4cp04569f

Elasticity tensor (kBar)[1]

10985.9067	383.6956	889.7178	-0.0000	0.0000	313.2885
383.6956	11582.6240	1002.7427	0.0000	-0.0000	-202.0731
889.7178	1002.7427	11527.7848	0.0000	-0.0000	-140.5836
-0.0000	0.0000	0.0000	4148.5658	-245.8980	0.0000
0.0000	-0.0000	-0.0000	-245.8980	5335.7938	-0.0000
313.2885	-202.0731	-140.5836	0.0000	-0.0000	4542.7086

[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].