SACADA Database Code: 207

Topology: 3^3,4T27

# of independent nodes (IN): 4
Transitivity: [4531]
Space Group: Cmcm
Pearson: oS28
Coordination Number (CN): 3, 4 (1:1)

Year: 2013

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
3^3,4T27 (SACADA #207)		1.545		0.646	161.1	81.2	10.5	SACADA[1]
ZGM-28		1.53	0.99					doi: 10.1002/adfm.201301077

Elasticity tensor (kBar)[1]

2184.6271	1831.9093	609.5272	0.0000	0.0000	-0.0000
1831.9093	1664.6756	488.6447	-0.0000	-0.0000	0.0000
609.5272	488.6447	7134.5287	0.0000	-0.0000	0.0000
0.0000	-0.0000	0.0000	1458.1242	0.0000	-0.0000
0.0000	-0.0000	-0.0000	0.0000	1419.3536	0.0000
-0.0000	0.0000	0.0000	-0.0000	-0.0000	1701.2235

[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].