SACADA Database Code: 192

Topology: $3,4^2T134$

# of independent nodes (IN): 3
Transitivity: [3894]
Space Group: Cmmm
Pearson: oS40
Coordination Number (CN): 3, 4 (2:3)

Year: 2013

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
$3,4^2T134$ (SACADA #192)		2.607		1.014	282.9	187.9	21.4	SACADA[1]
3D (5,0)-I	35		0.29					doi: 10.1038/srep01331

Elasticity tensor (kBar)[1]

3593.0962	865.5944	2625.3038	-0.0000	-0.0000	-0.0000
865.5944	8809.1137	1138.5703	-0.0000	0.0000	0.0000
2625.3038	1138.5703	4576.4517	-0.0000	0.0000	0.0000
-0.0000	-0.0000	0.0000	1997.6395	0.0000	-0.0000
-0.0000	-0.0000	0.0000	0.0000	3135.2730	0.0000
-0.0000	0.0000	0.0000	-0.0000	0.0000	1616.3914

[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].