SACADA Database Code: 162

Topology: $3,4^2T136$

# of independent nodes (IN): 3
Transitivity: [3442]
Space Group: Cmmm
Pearson: oS12
Coordination Number (CN): 3, 4 (1:2)

Year: 2011

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
$3,4^2T136$ (SACADA #162)		2.984		0.828	342.4	254.4	32.0	SACADA[1]
3D (3,3)		3.054			343.91	283.55	90.9	doi: 10.1021/nn202053t
3D (3,3)	35		1.24		343.91	283.55	90.9	doi: 10.1038/srep01331

Elasticity tensor (kBar)[1]

5010.8791	445.8780	1532.9213	-0.0000	0.0000	-0.0000
445.8780	11328.8018	1159.7372	-0.0000	-0.0000	-0.0000
1532.9213	1159.7372	10164.4665	0.0000	-0.0000	0.0000
-0.0000	-0.0000	0.0000	2207.8441	-0.0000	0.0000
0.0000	-0.0000	-0.0000	-0.0000	4439.9149	-0.0000
-0.0000	-0.0000	0.0000	0.0000	-0.0000	844.2812

[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].