SACADA Database Code: 165

Topology: $3,4^2T223$

# of independent nodes (IN): 3
Transitivity: [3454]
Space Group: P6/mmm
Pearson: hP18
Coordination Number (CN): 3, 4 (1:2)

Year: 2016

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
$3,4^2T223$ (SACADA #165)		3.189		0.936	355.2	339.5	59.2	SACADA[1]
H18		3.135	Metal		360	361		doi: 10.1038/srep21879

Elasticity tensor (kBar)[1]

11696.2992	1294.9799	387.1041	0.0000	0.0000	-0.0000
1294.9799	11696.2992	387.1041	-0.0000	-0.0000	-0.0000
387.1041	387.1041	6178.3453	0.0000	0.0000	-0.0000
0.0000	-0.0000	0.0000	5200.6597	-0.0000	0.0000
0.0000	-0.0000	0.0000	-0.0000	2089.1182	0.0000
-0.0000	-0.0000	-0.0000	0.0000	0.0000	2089.1182

[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].