SACADA Database Code: 76

Topology: tzs

# of independent nodes (IN): 1
Transitivity: [1343]
Space Group: I4/mcm
Pearson: tI16
Coordination Number (CN): 4

Year: 2004

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
tzs (SACADA #76)		3.158		0.323	387.2	369.5	64.3	SACADA[1]
3D (4,0)-I								doi: 10.1088/0953-8984/16/49/023
TA6								doi: 10.1134/s1063776111060173
TA6	35							link
3D (4,0)-I			2.81		391.51	379.90	89.9	doi: 10.1038/srep01331

Elasticity tensor (kBar)[1]

7304.1851	3673.7227	196.2923	-0.0000	0.0000	-0.0000
3673.7227	7304.1851	196.2923	0.0000	0.0000	0.0000
196.2923	196.2923	12169.4645	-0.0000	-0.0000	0.0000
0.0000	-0.0000	-0.0000	4559.3082	0.0000	0.0000
0.0000	0.0000	-0.0000	0.0000	3860.8592	0.0000
-0.0000	-0.0000	0.0000	0.0000	0.0000	3860.8592

[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].