SACADA Database Code: 276

Topology: 3^7T1

# of independent nodes (IN): 7
Transitivity: [7(11)62]
Space Group: Fd-3
Pearson: cF672
Coordination Number (CN): 3

Year: 1992

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
3^7T1 (SACADA #276)		1.271		0.112				SACADA[1]
D7'		1.28			115			doi: 10.1016/0008-6223(92)90066-6
C168					110			doi: 10.1103/PhysRevLett.68.511
D168								doi: 10.1103/PhysRevB.46.1941
D766								doi: 10.1016/0009-2614(93)85009-d
D7								doi: 10.1039/CS9952400341
D168								doi: 10.1021/jp9613201
D766								doi: 10.1016/s0960-8974(97)00003-x
D766								doi: 10.1088/1367-2630/5/1/126
super-cubic								doi: 10.1021/nl0622202
C-NT diamond-like								doi: 10.3103/s1063457610020012

[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].