SACADA Database Code: 93

Topology: xaa

# of independent nodes (IN): 2
Transitivity: [2223]
Space Group: Fm-3m
Pearson: cF80
Coordination Number (CN): 3

Year: 1998

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
xaa (SACADA #93)		2.114		0.918	237.9	29.3	4.8	SACADA[1]
C-20								doi: 10.1103/PhysRevB.58.664
C-20					247			doi: 10.1103/PhysRevB.78.125415
C-20		2.084	Metal					doi: 10.1039/c2cp43221h

Elasticity tensor (kBar)[1]

1343.3777	2896.9354	2896.9354	-0.0000	0.0000	0.0000
2896.9354	1343.3777	2896.9354	-0.0000	0.0000	-0.0000
2896.9354	2896.9354	1343.3777	0.0000	-0.0000	-0.0000
0.0000	-0.0000	0.0000	311.5993	0.0000	0.0000
0.0000	0.0000	-0.0000	0.0000	311.5993	0.0000
0.0000	-0.0000	-0.0000	0.0000	0.0000	311.5993

[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].