SACADA Database Code: 127

Topology: xca

# of independent nodes (IN): 2
Transitivity: [2443]
Space Group: Immm
Pearson: oI12
Coordination Number (CN): 3, 4 (1:2)

Year: 2005

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
xca (SACADA #127)		3.240		0.858	368.9	356.8	62.7	SACADA[1]
(4,0)	34		Metal		356			doi: 10.1103/PhysRevB.72.214109
3D-(4,0)		3.314			372.8	372.2	56.8	doi: 10.1021/nn202053t
(4,0)					373	372	60.6	doi: 10.1063/1.4952426

Elasticity tensor (kBar)[1]

12026.7767	1067.1745	780.0053	-0.0000	-0.0000	-0.0000
1067.1745	6068.0451	322.2138	0.0000	0.0000	-0.0000
780.0053	322.2138	12552.8735	0.0000	0.0000	-0.0000
-0.0000	0.0000	0.0000	2181.5549	0.0000	0.0000
-0.0000	0.0000	0.0000	0.0000	2456.3207	-0.0000
0.0000	0.0000	-0.0000	0.0000	-0.0000	5220.1045

[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].