SACADA Database Code: 133

Topology: sqc6952

# of independent nodes (IN): 2
Transitivity: [2465]
Space Group: P4/mmm
Pearson: tP16
Coordination Number (CN): 3, 4 (1:1)

Year: 2004

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
sqc6952 (SACADA #133)		2.705		1.106	274.8	197.6	23.8	SACADA[1]
(4,0)Dimer								doi: 10.1088/0953-8984/16/49/023
3D(4,0)-II			Metal		267.52	190.54	47.9	doi: 10.1038/srep01331

Elasticity tensor (kBar)[1]

4464.6724	2038.5409	799.3336	0.0000	-0.0000	0.0000
2038.5409	4464.6724	799.3336	-0.0000	-0.0000	0.0000
799.3336	799.3336	9045.0332	-0.0000	-0.0000	0.0000
0.0000	0.0000	0.0000	1435.4402	-0.0000	0.0000
-0.0000	-0.0000	-0.0000	-0.0000	2190.2613	-0.0000
0.0000	0.0000	-0.0000	0.0000	-0.0000	2190.2613

[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].

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