SACADA Database Code: 20

Topology: gsi

# of independent nodes (IN): 1
Transitivity: [1211]
Space Group: Ia-3
Pearson: cI16
Coordination Number (CN): 4

Year: 1984

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
gsi (SACADA #20)		3.621		1.243	408.3	535.4	102.4	SACADA[1]
BC-8	1200							doi: 10.1103/PhysRevB.30.3210
BC-8	1200		Metal		400.0			doi: 10.1103/PhysRevB.30.1773
BC-8								doi: 10.1103/PhysRevB.35.9559
BC-8		4.03	0.6					doi: 10.1021/ja00185a004
diam_cr44_ch*								doi: 10.1006/jssc.1999.8448
BC-8			2.4					doi: 10.1103/PhysRevB.59.733
BC-8								doi: 10.1007/978-94-010-1013-9_1
BC-8								doi: 10.1063/1.2210932
LA4								doi: 10.1134/s1063776111060173
BC-8								link
bc8			2.7		389.6		88.8	doi: 10.1103/PhysRevB.83.193410
BC-8			2.35		419.6	557.6	93.2	doi: 10.1021/ja304380p
LA4								link
BC-8								doi: 10.1002/pssb.201248185
gsi								doi: 10.1524/zkri.2013.1620
BC_8		3.558					88.6	doi: 10.1063/1.4794424
BC-8					386			doi: 10.1103/PhysRevB.91.214104
BC-8		3.556	3.58		372			doi: 10.1103/PhysRevB.91.214106
BC8					427	559		doi: 10.1038/srep21879

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
BC8		3.556						doi: 10.1088/0953-8984/28/47/475402
BC8		3.556			372			doi: 10.1103/PhysRevB.94.174102

Elasticity tensor (kBar)[1]

11469.1288	390.3507	390.3507	-0.0000	0.0000	0.0000
390.3507	11469.1288	390.3507	-0.0000	-0.0000	0.0000
390.3507	390.3507	11469.1288	-0.0000	-0.0000	0.0000
0.0000	-0.0000	-0.0000	5234.4515	0.0000	-0.0000
0.0000	-0.0000	-0.0000	0.0000	5234.4515	0.0000
0.0000	0.0000	0.0000	-0.0000	0.0000	5234.4515

[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].