SACADA Database Code: 141

Topology: sie

# of independent nodes (IN): 2
Transitivity: [2575]
Space Group: Cmmm
Pearson: oS16
Coordination Number (CN): 4

Year: 1997

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
sie (SACADA #141)		3.452		0.700	431.2	476.0	88.8	SACADA[1]
(RL)2								doi: 10.1016/S0379-6779(97)81165-4
oC16-II			3.15		408.4		84.4	doi: 10.1103/PhysRevB.84.161411
Cco-C8		3.51	3.12		444.1		95.1	doi: 10.1103/PhysRevLett.107.215502
Z-carbon		3.394	3.273		464.13		95.8	doi: 10.1016/j.ssc.2012.05.022
oCco-C8			3.09		433.4	486.9		doi: 10.1021/ja304380p
Z-carbon		3.399	3.273		415.83		81.09	doi: 10.1039/c2cp40531h
Z-carbon			4.7		441.5		95.4	doi: 10.1103/PhysRevLett.108.065501
Z-carbon								doi: 10.1021/ja301582d
Z-carbon								doi: 10.1063/1.4732136
oC16-II								doi: 10.1038/srep00471
Z-carbon								link
Z-carbon								doi: 10.1103/PhysRevB.85.155428
Z-carbon								doi: 10.1103/PhysRevB.85.144115
C8-carbon								doi: 10.3103/s1063457613010012
3D(2,2)-III			2.97		427.7	487.1	95.2	doi: 10.1038/srep01331
Z-carbon								doi: 10.1103/PhysRevB.88.014102
sie								doi: 10.1524/zkri.2013.1620
oC16-II								doi: 10.1002/zaac.201300652
Z-carbon					447			doi: 10.1016/j.carbon.2014.06.050

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
Cmmm					413			doi: 10.1103/PhysRevB.91.214104
Z-carbon								doi: 10.1088/0256-307x/32/9/096201
Z-carbon								doi: 10.1088/0253-6102/64/2/237
Z-carbon								doi: 10.1142/s0217984915300112
Z-carbon								doi: 10.1103/PhysRevB.93.085201

Elasticity tensor (kBar)[1]

11000.9475	812.5006	985.5628	0.0000	-0.0000	0.0000
812.5006	11396.9241	337.7158	0.0000	-0.0000	-0.0000
985.5628	337.7158	12161.6552	-0.0000	-0.0000	0.0000
-0.0000	0.0000	-0.0000	3600.4221	0.0000	-0.0000
-0.0000	-0.0000	-0.0000	0.0000	4583.4116	0.0000
0.0000	-0.0000	0.0000	-0.0000	0.0000	5099.5423

[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].