SACADA Database Code: 1

Topology: dia

# of independent nodes (IN): 1
Transitivity: [1111]
Space Group: Fd-3m
Pearson: cF8
Coordination Number (CN): 4

Year: 1913

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
dia (SACADA #1)		3.577		0.000	461.0	536.9	101.4	SACADA[1]
Diamond								doi: 10.1038/091557a0
Diamond		3.516						doi: 10.1006/jssc.1999.8448
Diamond		3.61						doi: 10.1016/S0009-2614(01)00126-9
Diamond					484	547		doi: 10.1088/1367-2630/5/1/123
Diamond		3.519	4.5		402.7			doi: 10.1103/PhysRevB.70.045101
Diamond					466			doi: 10.1103/PhysRevB.78.125415
Diamond		3.633			456.6	542.5		doi: 10.1021/nn202053t
Diamond			4.20		454.6	545.6	98.2	doi: 10.1021/ja304380p
LA1			5.37					link
Diamond		3.491			462.5			doi: 10.1063/1.4773584
Diamond			4.635					doi: 10.1039/c2cp43221h

Elasticity tensor (kBar)[1]

10845.0226	1493.1975	1493.1975	-0.0000	0.0000	0.0000
1493.1975	10845.0226	1493.1975	-0.0000	-0.0000	0.0000
1493.1975	1493.1975	10845.0226	0.0000	-0.0000	0.0000
-0.0000	-0.0000	0.0000	5888.1748	-0.0000	0.0000
0.0000	-0.0000	-0.0000	-0.0000	5888.1748	-0.0000
0.0000	0.0000	0.0000	-0.0000	-0.0000	5888.1748

[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].