SACADA Database Code: 70

Topology: unb

# of independent nodes (IN): 1
Transitivity: [1332]
Space Group: R-3m
Pearson: hR18
Coordination Number (CN): 4

Year: 2013

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
unb (SACADA #70)		3.346		0.563	177.1	203.8	38.4	SACADA[1]
unb								doi: 10.1524/zkri.2013.1620
LA9								doi: 10.1134/s1063776114060090
Rh6-II								doi: 10.1038/srep04339
Rh6-II								doi: 10.1186/s40679-016-0024-z
Rh6-II								doi: 10.1016/j.carbon.2016.02.056

Elasticity tensor (kBar)[1]

11269.6041	1397.2648	-331.1598	2.0047	642.0721	1.3859
1397.2648	11242.1198	-335.7461	0.5412	-639.6864	-0.7478
-331.1598	-335.7461	7918.3937	8.6056	7.2223	0.4411
2.0047	0.5412	8.6056	4939.4911	6.2760	639.8494
642.0721	-639.6864	7.2223	6.2760	2769.1432	3.9320
1.3859	-0.7478	0.4411	639.8494	3.9320	2768.0065

[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].