SACADA Database Code: 28

Topology: pcu-h (Allotrope with "sp" atoms)

# of independent nodes (IN): 3
Transitivity: [1221]
Space Group: R-3m
Pearson: hR54
Coordination Number (CN): 2, 3 (2:1)

Year: 2016

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
pcu-h (SACADA #28)		1.268		0.835	68.7	22.6	3.4	SACADA[1]
Rh18			0.58		129			doi: 10.1038/srep24665

Elasticity tensor (kBar)[1]

3561.9298	1944.2499	176.0152	-5.1529	174.4579	-7.1048
1944.2499	3619.7700	154.2518	3.7949	-183.6363	6.2778
176.0152	154.2518	65.3999	-5.6276	5.0953	-0.9767
-5.1529	3.7949	-5.6276	641.2424	1.2885	131.7457
174.4579	-183.6363	5.0953	1.2885	32.4285	-1.8581
-7.1048	6.2778	-0.9767	131.7457	-1.8581	21.0614

[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].