SACADA Database Code: 149

Topology: aht-3,4-Cmcm

# of independent nodes (IN): 2
Transitivity: -
Space Group: Cmcm
Pearson: oS24
Coordination Number (CN): 3, 4 (2:1)

Year: 2014

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
aht-3,4-Cmcm (SACADA #149)		2.448		0.791	205.9	148.9	18.1	SACADA[1]
oC24-carbon			Metal		225.6	178.2	27.6	doi: 10.3103/s1063457614040042
oC24-carbon								doi: 10.1002/pssb.201552234

Elasticity tensor (kBar)[1]

5690.7746	2465.3405	1492.5470	0.0000	0.0000	0.0000
2465.3405	1632.1335	557.3175	-0.0000	-0.0000	0.0000
1492.5470	557.3175	9721.0863	0.0000	-0.0000	-0.0000
0.0000	-0.0000	-0.0000	1310.1856	0.0000	-0.0000
0.0000	0.0000	0.0000	0.0000	1503.5645	0.0000
-0.0000	0.0000	-0.0000	-0.0000	0.0000	3710.5592

[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].