SACADA Database Code: 448

Topology: nbo-x-d-4,4-C2/m-2

# of independent nodes (IN): 2
Transitivity: [2451]
Space Group: I2/m
Pearson: mS10
Coordination Number (CN): 4

Year: 2017

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
nbo-x-d-4,4-C2/m-2 (SACADA #448)		3.213		1.412	-	-	-	SACADA[1]
G154								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

5506.0921	877.1278	2538.1821	0.0000	-0.0000	-1430.6323
877.1278	9455.1530	21.3975	-0.0000	0.0000	-342.1346
2538.1821	21.3975	6523.6386	-0.0000	0.0000	850.4886
0.0000	-0.0000	-0.0000	-1298.9979	2404.8345	0.0000
0.0000	0.0000	0.0000	2404.8345	413.0896	-0.0000
-1430.6323	-342.1346	850.4886	0.0000	-0.0000	2297.3670

[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].