SACADA Database Code: 368

Topology: noq

# of independent nodes (IN): 2
Transitivity: [2441]
Space Group: C2/c
Pearson: mS12
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
noq (SACADA #368)		3.186		1.119	349.9	334.2	58.2	SACADA[1]
G26								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

8841.2979	1866.0072	1236.0813	-0.0000	0.0000	114.0756
1866.0072	6225.6936	708.4106	0.0000	-0.0000	445.1710
1236.0813	708.4106	9286.1452	0.0000	-0.0000	-931.4036
-0.0000	0.0000	0.0000	2760.3528	-140.2504	-0.0000
0.0000	-0.0000	-0.0000	-140.2504	3113.1084	0.0000
114.0756	445.1710	-931.4036	-0.0000	0.0000	4350.9836

[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].