SACADA Database Code: 476

Topology: 4^3T181

# of independent nodes (IN): 3
Transitivity: [3763]
Space Group: C2/c
Pearson: mS24
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
4^3T181 (SACADA #476)		3.323		0.994	369.5	396.6	73.4	SACADA[1]
G184								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

9781.0185	1113.5317	700.4480	-0.0000	-0.0000	-525.1872
1113.5317	9272.7492	512.3681	-0.0000	-0.0000	531.9750
700.4480	512.3681	9566.1665	-0.0000	-0.0000	-101.6177
-0.0000	-0.0000	-0.0000	4263.8821	-55.1226	0.0000
-0.0000	-0.0000	0.0000	-55.1226	2866.3989	-0.0000
-525.1872	531.9750	-101.6177	0.0000	-0.0000	4210.3667

[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].