SACADA Database Code: 466

Topology: 4^8T42

# of independent nodes (IN): 8
Transitivity: [8(16)(13)5]
Space Group: Cc
Pearson: mS32
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
4^8T42 (SACADA #466)		3.418		0.945	400.0	443.5	82.9	SACADA[1]
G174								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

10381.0759	1177.4502	648.6983	-0.0000	0.0000	249.4617
1177.4502	10396.6275	806.8850	-0.0000	0.0000	74.3390
648.6983	806.8850	9985.6106	-0.0000	0.0000	-71.0195
-0.0000	-0.0000	-0.0000	4481.2131	-149.7456	0.0000
0.0000	0.0000	0.0000	-149.7456	4467.5288	-0.0000
249.4617	74.3390	-71.0195	0.0000	-0.0000	3901.6100

[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].