SACADA Database Code: 483

Topology: 4^6T41

# of independent nodes (IN): 6
Transitivity: [6(12)(10)5]
Space Group: C2
Pearson: mS20
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
4^6T41 (SACADA #483)		3.274		1.209	365.8	367.7	66.2	SACADA[1]
G191								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

9859.2246	826.3119	796.7838	0.0000	-0.0000	384.1477
826.3119	8070.3709	1795.0358	-0.0000	0.0000	-175.0126
796.7838	1795.0358	8177.6994	0.0000	-0.0000	218.0405
0.0000	-0.0000	0.0000	3723.6756	222.3873	0.0000
-0.0000	0.0000	0.0000	222.3873	3398.3445	0.0000
384.1477	-175.0126	218.0405	0.0000	0.0000	3816.1068

[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].