SACADA Database Code: 486

Topology: 4^7T28

# of independent nodes (IN): 7
Transitivity: [7(12)(13)7]
Space Group: C2
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
4^7T28 (SACADA #486)		3.342		1.179	351.5	374.3	69.1	SACADA[1]
G195								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

9830.1200	965.9460	670.9098	-0.0000	-0.0000	432.7854
965.9460	8678.6856	1353.0152	0.0000	-0.0000	-104.9266
670.9098	1353.0152	7318.8269	-0.0000	0.0000	517.0577
-0.0000	0.0000	-0.0000	4591.7421	211.3359	-0.0000
-0.0000	-0.0000	0.0000	211.3359	3908.8598	0.0000
432.7854	-104.9266	517.0577	-0.0000	0.0000	2892.0984

[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].