SACADA Database Code: 478

Topology: 4^7T27

# of independent nodes (IN): 7
Transitivity: [7(14)(13)5]
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
4^7T27 (SACADA #478)		3.343		1.030	371.2	406.1	75.6	SACADA[1]
G186								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

9633.7591	695.3271	1365.1760	0.0000	-0.0000	156.1837
695.3271	8527.2240	1061.6098	0.0000	-0.0000	-364.6046
1365.1760	1061.6098	9072.6130	-0.0000	0.0000	227.3819
0.0000	0.0000	-0.0000	3818.1612	-7.4544	0.0000
-0.0000	-0.0000	0.0000	-7.4544	3973.2043	-0.0000
156.1837	-364.6046	227.3819	0.0000	-0.0000	4529.3692

[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].