SACADA Database Code: 499

Topology: 4^7T29

# of independent nodes (IN): 7
Transitivity: [7(14)(12)5]
Space Group: P21
Pearson: mP14
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
4^7T29 (SACADA #499)		3.264		1.074	363.4	376.6	68.8	SACADA[1]
G212								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

8728.8877	958.8518	1672.9016	-0.0001	-0.0000	-52.0244
958.8518	9270.9511	718.9108	-0.0001	-0.0001	-99.9593
1672.9016	718.9108	8035.0367	-0.0000	-0.0001	103.0274
-0.0001	-0.0001	-0.0000	4114.5602	-456.9449	-0.0000
-0.0000	-0.0001	-0.0001	-456.9449	3335.5310	-0.0000
-52.0244	-99.9593	103.0274	-0.0000	-0.0000	3919.6849

[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].