SACADA Database Code: 487

Topology: 4^6T42

# of independent nodes (IN): 6
Transitivity: [6(14)(10)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
4^6T42 (SACADA #487)		3.281		1.163	348.6	353.6	63.9	SACADA[1]
G196								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

9451.0577	942.4307	690.7225	-0.0000	0.0000	-97.9009
942.4307	8721.3120	443.8363	-0.0000	0.0000	-256.0673
690.7225	443.8363	9084.1698	0.0000	0.0000	208.7573
-0.0000	-0.0000	0.0000	3319.7878	-241.5673	-0.0000
0.0000	-0.0000	0.0000	-241.5673	2784.7757	0.0000
-97.9009	-256.0673	208.7573	-0.0000	0.0000	3401.5733

[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].