SACADA Database Code: 475

Topology: 4^7T26

# of independent nodes (IN): 7
Transitivity: [7(12)72]
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
4^7T26 (SACADA #475)		3.352		1.079	378.1	397.4	73.0	SACADA[1]
G183								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

8854.5865	889.8379	1594.6151	-0.0000	0.0000	59.8664
889.8379	10073.4507	870.1746	0.0000	-0.0000	15.7212
1594.6151	870.1746	8419.6856	0.0000	0.0000	-28.6764
-0.0000	0.0000	-0.0000	4004.0729	-254.6538	0.0000
0.0000	-0.0000	0.0000	-254.6538	3869.9228	0.0000
59.8664	15.7212	-28.6764	-0.0000	0.0000	4058.5630

[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].