SACADA Database Code: 425

Topology: 4^9T7

# of independent nodes (IN): 9
Transitivity: [9(17)(14)6]
Space Group: C2
Pearson: mS32
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
4^9T7 (SACADA #425)		3.397		0.813	397.4	436.1	81.3	SACADA[1]
G125								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

10154.9231	1223.5892	1207.9141	0.0000	-0.0000	-385.3898
1223.5892	8902.6233	1377.4956	0.0000	-0.0000	84.3130
1207.9141	1377.4956	9123.9322	-0.0000	-0.0000	284.4067
0.0000	0.0000	-0.0000	4366.5831	57.5304	-0.0000
-0.0000	-0.0000	-0.0000	57.5304	4531.8828	-0.0000
-385.3898	84.3130	284.4067	-0.0000	-0.0000	4858.3667

[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].