SACADA Database Code: 430

Topology: 4^8T36

# of independent nodes (IN): 8
Transitivity: [8(17)(13)5]
Space Group: I2
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
4^8T36 (SACADA #430)		3.279		1.007	367.8	382.1	69.9	SACADA[1]
G130								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

8806.3705	1425.3223	1033.4444	0.0000	-0.0000	331.6914
1425.3223	8214.7994	754.7781	-0.0000	0.0000	-33.7192
1033.4444	754.7781	9697.8814	-0.0000	0.0000	96.4433
-0.0000	-0.0000	-0.0000	3943.8349	33.0683	-0.0000
-0.0000	0.0000	0.0000	33.0683	3525.7171	-0.0000
331.6914	-33.7192	96.4433	-0.0000	0.0000	3859.0117

[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].