SACADA Database Code: 409

Topology: 4^5T55

# of independent nodes (IN): 5
Transitivity: [5894]
Space Group: C2/m
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
4^5T55 (SACADA #409)		3.211		1.177	347.6	306.8	49.6	SACADA[1]
G103								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

7179.8946	1200.4331	2158.6216	0.0000	-0.0000	-189.7480
1200.4331	6794.2227	1078.9829	-0.0000	0.0000	-142.6293
2158.6216	1078.9829	8754.0069	-0.0000	0.0000	-597.1227
0.0000	-0.0000	0.0000	3307.8101	-153.8390	0.0000
-0.0000	0.0000	0.0000	-153.8390	2603.4926	-0.0000
-189.7480	-142.6293	-597.1227	0.0000	-0.0000	3462.0274

[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].