SACADA Database Code: 514

Topology: 4^4T124

# of independent nodes (IN): 4
Transitivity: [4764]
Space Group: Cmcm
Pearson: oS24
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
4^4T124 (SACADA #514)		3.251		0.870	374.5	393.2	72.2	SACADA[1]
G229								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

9978.0860	1585.5742	376.8973	0.0000	-0.0000	-0.0000
1585.5742	7993.8646	743.9998	0.0000	-0.0000	0.0000
376.8973	743.9998	10417.4698	-0.0000	-0.0000	-0.0000
-0.0000	-0.0000	0.0000	3115.1514	0.0000	0.0000
-0.0000	-0.0000	-0.0000	0.0000	4407.5262	-0.0000
-0.0000	0.0000	-0.0000	0.0000	-0.0000	3850.7573

[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].