SACADA Database Code: 408

Topology: 4^2T263

# of independent nodes (IN): 2
Transitivity: [2473]
Space Group: Cccm
Pearson: oS20
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
4^2T263 (SACADA #408)		3.256		1.381	362.8	321.3	52.2	SACADA[1]
G102								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

11005.1910	733.4659	387.6688	2.5073	1.0282	1.3609
733.4659	7026.4283	2193.0217	5.4219	0.1920	-1.2524
387.6688	2193.0217	8140.4794	8.9310	-1.6511	0.1723
2.5073	5.4219	8.9310	4771.3330	4.2432	1.4308
1.0282	0.1920	-1.6511	4.2432	3011.2797	6.4970
1.3609	-1.2524	0.1723	1.4308	6.4970	1806.4816

[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].