SACADA Database Code: 496

Topology: 4^4T122

# of independent nodes (IN): 4
Transitivity: [4972]
Space Group: P2/m1
Pearson: mP16
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
4^4T122 (SACADA #496)		3.403		0.881	415.6	452.9	84.2	SACADA[1]
G208								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

9152.4444	1524.3722	1298.0167	3.6973	2.2729	79.5677
1524.3722	10174.2090	665.2004	-0.1603	-1.1163	34.0255
1298.0167	665.2004	11145.3910	5.3593	0.4144	461.1777
3.6973	-0.1603	5.3593	4350.5312	-137.4240	-3.4315
2.2729	-1.1163	0.4144	-137.4240	4253.3473	0.7494
79.5677	34.0255	461.1777	-3.4315	0.7494	5167.3390

[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].