SACADA Database Code: 494

Topology: 4^8T17

# of independent nodes (IN): 8
Transitivity: [8(18)(11)4]
Space Group: P-1
Pearson: aP16
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
4^8T17 (SACADA #494)		3.276		0.761	391.3	411.6	75.6	SACADA[1]
G206								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

8676.1681	1541.1204	1155.9852	-8.4192	15.9924	-13.9489
1541.1204	8878.3756	1370.4752	23.6010	141.2984	-53.3957
1155.9852	1370.4752	9548.2871	-65.7655	-298.4777	-17.3889
-8.4192	23.6010	-65.7655	4519.6028	116.5404	-96.9394
15.9924	141.2984	-298.4777	116.5404	3829.5437	80.0985
-13.9489	-53.3957	-17.3889	-96.9394	80.0985	4668.5922

[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].