SACADA Database Code: 401

Topology: 4^8T29

# of independent nodes (IN): 8
Transitivity: [8(16)(16)8]
Space Group: P21
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
4^8T29 (SACADA #401)		3.532		0.771	423.5	501.2	94.9	SACADA[1]
G92								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

11661.4814	472.7816	435.9256	0.0001	0.0000	45.0933
472.7816	12012.7396	770.8298	0.0001	0.0001	-20.0430
435.9256	770.8298	11100.1679	0.0000	0.0001	-136.4290
0.0001	0.0001	0.0000	4866.0769	-153.3200	0.0000
0.0000	0.0001	0.0001	-153.3200	5053.2821	0.0000
45.0933	-20.0430	-136.4290	0.0000	0.0000	4235.1818

[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].