SACADA Database Code: 457

Topology: 4^2T266

# of independent nodes (IN): 2
Transitivity: [2772]
Space Group: Imma
Pearson: oI32
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
4^2T266 (SACADA #457)		3.195		0.964	367.4	354.4	62.2	SACADA[1]
G164								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

7954.6713	1575.0888	1894.3117	0.0000	0.0000	-0.0000
1575.0888	8848.6780	459.3260	-0.0000	-0.0000	-0.0000
1894.3117	459.3260	8425.4142	-0.0000	-0.0000	0.0000
0.0000	-0.0000	-0.0000	3107.7610	-0.0000	0.0000
0.0000	-0.0000	-0.0000	-0.0000	3813.6983	-0.0000
-0.0000	0.0000	0.0000	0.0000	-0.0000	3840.9840

[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].