SACADA Database Code: 397

Topology: 4^3T144

# of independent nodes (IN): 3
Transitivity: [3895]
Space Group: Immm
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
4^3T144 (SACADA #397)		3.341		0.803	391.0	422.5	78.4	SACADA[1]
G88								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

10836.5364	579.5332	261.4772	-0.0000	0.0000	-0.0000
579.5332	10399.3331	1093.2008	-0.0000	-0.0000	-0.0000
261.4772	1093.2008	10095.7602	-0.0000	0.0000	0.0000
-0.0000	-0.0000	-0.0000	3597.3230	0.0000	-0.0000
0.0000	-0.0000	0.0000	0.0000	4208.5773	-0.0000
-0.0000	-0.0000	0.0000	-0.0000	-0.0000	3719.3640

[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].