SACADA Database Code: 406

Topology: 4^2T262

# of independent nodes (IN): 2
Transitivity: [2663]
Space Group: Cmcm
Pearson: oS24
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
4^2T262 (SACADA #406)		3.230		0.902	369.0	387.6	71.2	SACADA[1]
G99								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

10643.0598	771.7171	780.9112	0.0000	-0.0000	-0.0000
771.7171	9478.8876	56.6923	-0.0000	-0.0000	0.0000
780.9112	56.6923	9973.4172	-0.0000	0.0000	0.0000
0.0000	-0.0000	-0.0000	3218.5577	0.0000	0.0000
-0.0000	-0.0000	0.0000	0.0000	3681.4150	-0.0000
0.0000	0.0000	0.0000	0.0000	-0.0000	3282.0517

[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].