SACADA Database Code: 387

Topology: 4^2T261

# of independent nodes (IN): 2
Transitivity: [2783]
Space Group: Cmcm
Pearson: oS32
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
4^2T261 (SACADA #387)		3.282		0.897	376.1	397.5	73.2	SACADA[1]
G76								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

9432.5983	1912.4381	781.8843	0.0000	-0.0000	-0.0004
1912.4381	8570.0430	57.1361	-0.0000	-0.0000	-0.0000
781.8843	57.1361	10435.1353	-0.0000	-0.0000	-0.0005
0.0000	-0.0000	-0.0000	4030.8037	-0.0002	0.0000
-0.0000	-0.0000	-0.0000	-0.0002	3833.8898	0.0000
-0.0004	-0.0000	-0.0005	0.0000	0.0000	3613.2421

[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].