SACADA Database Code: 442

Topology: 4^2T265

# of independent nodes (IN): 2
Transitivity: [2652]
Space Group: C2/c
Pearson: mS16
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
4^2T265 (SACADA #442)		3.404		1.032	385.0	421.1	78.4	SACADA[1]
G147								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

8144.1819	1801.7482	791.7313	0.0000	-0.0000	303.2572
1801.7482	9266.3339	496.2134	0.0000	-0.0000	176.2632
791.7313	496.2134	11139.3292	-0.0000	0.0000	215.9896
0.0000	0.0000	0.0000	4579.2597	580.6391	-0.0000
-0.0000	-0.0000	0.0000	580.6391	3973.5085	0.0000
303.2572	176.2632	215.9896	-0.0000	0.0000	4216.7467

[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].