SACADA Database Code: 362

Topology: 4^8T21

# of independent nodes (IN): 8
Transitivity: [8(16)91]
Space Group: P1
Pearson: aP8
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
4^8T21 (SACADA #362)		3.267		1.013	368.0	375.5	68.1	SACADA[1]
G13								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

8557.6941	1028.8875	1258.5452	9.2513	-7.1411	-152.4635
1028.8875	9735.4484	1023.9161	-132.9693	-7.2304	53.5912
1258.5452	1023.9161	8265.1789	-13.7905	211.3277	-229.8163
9.2513	-132.9693	-13.7905	3507.3643	261.5038	-171.5301
-7.1411	-7.2304	211.3277	261.5038	3591.2247	194.4886
-152.4635	53.5912	-229.8163	-171.5301	194.4886	3989.6656

[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].