SACADA Database Code: 427

Topology: 4^8T35

# of independent nodes (IN): 8
Transitivity: [8(17)(13)5]
Space Group: P-1
Pearson: aP16
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
4^8T35 (SACADA #427)		3.307		1.164	346.4	355.2	64.6	SACADA[1]
G127								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

8957.8329	1273.2896	661.3677	171.5987	-58.4148	-102.4611
1273.2896	8033.2070	405.3608	475.1273	-197.1905	184.5127
661.3677	405.3608	9588.6276	-69.6128	-135.7504	-237.3298
171.5987	475.1273	-69.6128	3568.7392	-131.6844	-502.4909
-58.4148	-197.1905	-135.7504	-131.6844	2914.4781	26.7260
-102.4611	184.5127	-237.3298	-502.4909	26.7260	3448.6081

[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].