SACADA Database Code: 456

Topology: 4^8T40

# of independent nodes (IN): 8
Transitivity: [8(18)(13)6]
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
4^8T40 (SACADA #456)		3.387		0.837	400.5	431.0	79.9	SACADA[1]
G163								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

8897.9005	1485.5413	1366.1556	-110.2789	298.1477	97.2494
1485.5413	9294.3401	1074.6064	-190.3997	-276.5703	3.9791
1366.1556	1074.6064	10026.6703	221.9427	-276.4658	142.0885
-110.2789	-190.3997	221.9427	4376.3774	427.8246	-24.5993
298.1477	-276.5703	-276.4658	427.8246	4553.2259	-209.5850
97.2494	3.9791	142.0885	-24.5993	-209.5850	4610.6790

[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].