SACADA Database Code: 468

Topology: 4^8T43

# of independent nodes (IN): 8
Transitivity: [8(16)(10)2]
Space Group: An
Pearson: mS32
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
4^8T43 (SACADA #468)		3.393		0.882	394.5	435.5	81.3	SACADA[1]
G176								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

10262.8356	621.7254	1268.3299	-0.0366	-1.7059	-381.0623
621.7254	9372.2501	944.2991	2.5572	1.4534	513.1356
1268.3299	944.2991	10272.9935	8.0375	2.3770	336.4661
-0.0366	2.5572	8.0375	3645.7409	467.4685	0.1355
-1.7059	1.4534	2.3770	467.4685	4402.2194	3.3977
-381.0623	513.1356	336.4661	0.1355	3.3977	4811.7268

[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].