SACADA Database Code: 363

Topology: 4^{14}T2

# of independent nodes (IN): 14
Transitivity: [(14)(21)(19)(12)]
Space Group: Cm
Pearson: mS28
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^{14}T2 (SACADA #363)		3.417		0.679	408.8	468.2	88.2	SACADA[1]
G14								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

11395.4113	382.9963	710.0108	-0.0000	-0.0000	322.3853
382.9963	11098.1673	888.4504	-0.0000	0.0000	-158.4944
710.0108	888.4504	10341.8307	0.0000	-0.0000	-52.9915
-0.0000	-0.0000	0.0000	4495.1896	-157.2634	0.0000
-0.0000	0.0000	-0.0000	-157.2634	4854.6530	0.0000
322.3853	-158.4944	-52.9915	0.0000	0.0000	3915.3275

[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].