SACADA Database Code: 589

Topology: 4^3T165-CA

# of independent nodes (IN): 3
Transitivity: [3642]
Space Group: Cmcm
Pearson: oS24
Coordination Number (CN): 4

Year: 2021

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^3T165-CA (SACADA #589)		2.680		0.916	250.4	179.9	21.7	SACADA[1]
4^3T165-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

9349.3983	36.0704	175.0903	-0.0000	0.0000	0.0000
36.0704	3408.0102	2616.1748	-0.0000	0.0000	0.0000
175.0903	2616.1748	4933.3462	0.0000	-0.0000	-0.0000
-0.0000	-0.0000	0.0000	2799.1809	0.0000	-0.0000
0.0000	0.0000	-0.0000	0.0000	1018.1620	-0.0000
0.0000	0.0000	-0.0000	0.0000	-0.0000	1986.7306

[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].