SACADA Database Code: 612

Topology: 4^3T189-CA

# of independent nodes (IN): 3
Transitivity: [3884]
Space Group: Cmmm
Pearson: oS32
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
4^3T189-CA (SACADA #612)		2.829		0.819	285.5	192.1	22.0	SACADA[1]
4^3T189-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

4361.2661	1395.6176	1380.2884	0.0000	0.0000	-0.0000
1395.6176	5171.1801	1826.5479	-0.0000	-0.0000	0.0000
1380.2884	1826.5479	7729.3803	-0.0000	-0.0000	0.0000
0.0000	-0.0000	-0.0000	1864.9609	0.0000	-0.0000
0.0000	-0.0000	-0.0000	0.0000	2141.9067	-0.0000
-0.0000	0.0000	0.0000	-0.0000	-0.0000	1566.1049

[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].