SACADA Database Code: 579

Topology: 4^3T154-CA

# of independent nodes (IN): 3
Transitivity: [3762]
Space Group: I2/c
Pearson: mS24
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
4^3T154-CA (SACADA #579)		3.552		1.135	388.9	427.0	79.6	SACADA[1]
4^3T154-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

6862.4008	55.3587	1850.6877	-0.0000	0.0000	-328.8465
55.3587	14557.5980	599.9289	-0.0000	0.0000	-137.6855
1850.6877	599.9289	9670.3544	-0.0000	0.0000	-328.3819
-0.0000	-0.0000	-0.0000	3730.5417	-347.1487	0.0000
0.0000	0.0000	0.0000	-347.1487	5042.6160	-0.0000
-328.8465	-137.6855	-328.3819	0.0000	-0.0000	3818.7361

[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].