SACADA Database Code: 490

Topology: 4^4T120

# of independent nodes (IN): 4
Transitivity: [4564]
Space Group: Cmmm
Pearson: oS20
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
4^4T120 (SACADA #490)		3.267		1.649	-	-	-	SACADA[1]
G199								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

6633.5222	1569.2925	661.5443	0.0000	0.0000	-0.0000
1569.2925	9295.6180	1180.8792	0.0000	0.0000	-0.0000
661.5443	1180.8792	8870.1967	0.0000	-0.0000	0.0000
-0.0000	0.0000	0.0000	-2668.7598	0.0000	-0.0000
0.0000	0.0000	-0.0000	0.0000	2814.6200	0.0000
-0.0000	-0.0000	0.0000	-0.0000	0.0000	2140.9466

[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].