SACADA Database Code: 395

Topology: 4^5T52

# of independent nodes (IN): 5
Transitivity: [5(10)(10)5]
Space Group: C2221
Pearson: oS32
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
4^5T52 (SACADA #395)		3.517		0.825	410.5	477.5	90.2	SACADA[1]
G86								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

9599.4804	1602.4268	815.4782	-0.0000	0.0000	-0.0000
1602.4268	10230.1200	400.1013	0.0000	0.0000	0.0000
815.4782	400.1013	11486.7241	-0.0000	0.0000	-0.0000
-0.0000	-0.0000	-0.0000	4980.6034	-0.0000	-0.0000
0.0000	0.0000	0.0000	0.0000	4419.1043	-0.0000
-0.0000	0.0000	-0.0000	-0.0000	-0.0000	5093.0313

[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].