SACADA Database Code: 200

Topology: 3^2,4T206

# of independent nodes (IN): 3
Transitivity: -
Space Group: P3212
Pearson: hP18
Coordination Number (CN): 3, 4 (2:1)

Year: 2015

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
3^2,4T206 (SACADA #200)		2.445		0.813	277.2	227.2	33.2	SACADA[1]
Tri-C18	0-20	2.494	Metal		276.5	236.8	37.0	doi: 10.1016/j.carbon.2015.05.027

Elasticity tensor (kBar)[1]

4754.6655	1577.2220	633.6503	2.7210	4.3073	4.5558
1577.2220	4778.2334	623.4909	-1.6847	-1.3780	-5.1545
633.6503	623.4909	10749.2559	0.1065	1.8736	0.2313
2.7210	-1.6847	0.1065	1604.4827	-8.1894	-0.8330
4.3073	-1.3780	1.8736	-8.1894	2350.6843	-0.6807
4.5558	-5.1545	0.2313	-0.8330	-0.6807	2346.7859

[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].