SACADA Database Code: 122

Topology: 4^2T63

# of independent nodes (IN): 2
Transitivity: [2422]
Space Group: R-3
Pearson: hR24
Coordination Number (CN): 4

Year: 2015

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^2T63 (SACADA #122)		3.596		1.362	385.5	500.9	95.8	SACADA[1]
r8					363			doi: 10.1103/PhysRevB.91.214104
r8		3.532			348			doi: 10.1103/PhysRevB.94.174102

Elasticity tensor (kBar)[1]

11237.5933	314.4869	603.8883	-0.0000	231.5013	35.6303
314.4869	11237.5933	603.8883	-0.0000	-231.5013	-35.6303
603.8883	603.8883	9274.3749	-0.0004	-0.0000	-0.0000
-0.0000	-0.0000	-0.0004	5461.5532	-35.6303	231.5013
231.5013	-231.5013	-0.0000	-35.6303	4802.9756	-0.0000
35.6303	-35.6303	-0.0000	231.5013	-0.0000	4802.9756

[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].