SACADA Database Code: 391

Topology: 4^2T193

# of independent nodes (IN): 2
Transitivity: [2543]
Space Group: I41/a
Pearson: tI32
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
4^2T193 (SACADA #391)		3.395		0.844	398.5	441.5	82.5	SACADA[1]
G80								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

10084.8962	1110.5921	1071.5401	-672.5407	-0.0000	0.0000
1110.5921	10084.8962	1071.5401	672.5407	-0.0000	-0.0000
1071.5401	1071.5401	9224.4070	0.0000	0.0000	0.0000
-672.5407	672.5407	0.0000	4849.7553	-0.0000	-0.0000
-0.0000	-0.0000	0.0000	-0.0000	4271.5186	-0.0000
0.0000	-0.0000	-0.0000	-0.0000	-0.0000	4271.5186

[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].