SACADA Database Code: 493

Topology: 4^8T47

# of independent nodes (IN): 8
Transitivity: [8(13)(11)6]
Space Group: P21/m
Pearson: mP16
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
4^8T47 (SACADA #493)		3.366		0.822	390.2	416.9	77.0	SACADA[1]
G205								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

10755.9170	623.4229	994.9478	-0.0000	-0.0000	-204.8478
623.4229	10699.3127	598.9951	-0.0000	0.0000	220.1143
994.9478	598.9951	9296.7758	-0.0000	-0.0000	-263.6163
-0.0000	-0.0000	-0.0000	4400.9522	130.2136	0.0000
-0.0000	0.0000	-0.0000	130.2136	3863.2087	0.0000
-204.8478	220.1143	-263.6163	0.0000	0.0000	3295.1143

[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].