SACADA Database Code: 390

Topology: 4^8T24

# of independent nodes (IN): 8
Transitivity: [8(17)(17)8]
Space Group: C2
Pearson: mS32
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
4^8T24 (SACADA #390)		3.528		0.753	420.5	493.0	93.2	SACADA[1]
G79								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

11115.2963	567.5083	655.8788	-0.0000	-0.0000	-106.6843
567.5083	11747.9428	804.0227	-0.0000	0.0000	-249.0551
655.8788	804.0227	10946.7827	0.0000	0.0000	334.5270
-0.0000	-0.0000	0.0000	4739.7972	-354.8912	0.0000
-0.0000	-0.0000	0.0000	-354.8912	5111.9078	-0.0000
-106.6843	-249.0551	334.5270	0.0000	-0.0000	4290.3191

[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].