SACADA Database Code: 400

Topology: 4^8T28

# of independent nodes (IN): 8
Transitivity: [8(17)(13)6]
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
4^8T28 (SACADA #400)		3.332		0.875	377.4	413.9	77.1	SACADA[1]
G91								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

9637.5979	1334.0135	1070.7908	0.0000	-0.0000	90.5360
1334.0135	8329.6105	587.5379	0.0000	-0.0000	403.6313
1070.7908	587.5379	10129.3751	0.0000	-0.0000	-541.6851
0.0000	0.0000	0.0000	4248.9559	147.2297	-0.0000
-0.0000	-0.0000	-0.0000	147.2297	3660.2768	0.0000
90.5360	403.6313	-541.6851	-0.0000	0.0000	4511.9301

[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].