SACADA Database Code: 385

Topology: 4^8T23

# of independent nodes (IN): 8
Transitivity: [8(15)(11)5]
Space Group: C2
Pearson: mS28
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
4^8T23 (SACADA #385)		3.407		0.881	397.9	450.1	84.5	SACADA[1]
G69								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

9726.5046	1244.3727	1020.3263	-0.0000	-0.0000	264.8347
1244.3727	9355.3369	1224.0865	-0.0000	-0.0000	-103.7522
1020.3263	1224.0865	9753.7347	-0.0000	-0.0000	672.2014
-0.0000	-0.0000	-0.0000	4807.0446	8.5764	-0.0000
-0.0000	-0.0000	-0.0000	8.5764	4670.6326	-0.0000
264.8347	-103.7522	672.2014	-0.0000	-0.0000	4617.8079

[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].