SACADA Database Code: 484

Topology: 4^8T46

# of independent nodes (IN): 8
Transitivity: [8(15)(15)8]
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
4^8T46 (SACADA #484)		3.401		1.060	379.5	413.7	76.9	SACADA[1]
G193								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

8581.0383	1509.2779	1258.1716	0.0000	-0.0000	160.0365
1509.2779	8464.8330	1277.2044	-0.0000	-0.0000	6.1463
1258.1716	1277.2044	9030.3942	-0.0000	0.0000	-208.9474
0.0000	-0.0000	-0.0000	4315.9971	50.0548	-0.0000
-0.0000	-0.0000	0.0000	50.0548	4456.9465	-0.0000
160.0365	6.1463	-208.9474	-0.0000	-0.0000	4684.9819

[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].