SACADA Database Code: 439

Topology: 4^6T34

# of independent nodes (IN): 6
Transitivity: [6(13)(13)4]
Space Group: P-1
Pearson: aP12
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
4^6T34 (SACADA #439)		3.360		1.143	359.0	386.1	71.5	SACADA[1]
G142								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

10689.6027	673.9238	931.3330	-750.9313	103.6396	109.8196
673.9238	8934.7323	1064.6977	-58.1832	4.7508	-36.9171
931.3330	1064.6977	7573.5199	152.5342	-234.7017	-384.1332
-750.9313	-58.1832	152.5342	4567.4348	-57.6447	86.4838
103.6396	4.7508	-234.7017	-57.6447	2703.4038	106.9869
109.8196	-36.9171	-384.1332	86.4838	106.9869	4308.7211

[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].