SACADA Database Code: 520

Topology: 4^6T48

# of independent nodes (IN): 6
Transitivity: [6996]
Space Group: C2221
Pearson: oS32
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
4^6T48 (SACADA #520)		3.310		0.751	395.5	425.6	78.9	SACADA[1]
G241								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

9037.0159	1450.1233	1471.9511	0.0000	0.0000	0.0000
1450.1233	9963.8548	1050.1305	-0.0000	0.0002	-0.0000
1471.9511	1050.1305	8700.8192	-0.0000	0.0002	-0.0000
-0.0000	-0.0000	0.0000	3701.1158	0.0000	0.0001
0.0000	0.0002	0.0002	0.0000	5013.9591	0.0000
0.0000	-0.0000	-0.0000	0.0001	0.0000	4840.3471

[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].