SACADA Database Code: 497

Topology: 4^4T123

# of independent nodes (IN): 4
Transitivity: [4(10)85]
Space Group: C2/c
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
4^4T123 (SACADA #497)		3.431		1.006	374.0	435.9	82.3	SACADA[1]
G209								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

9284.6790	1514.0181	842.1369	0.0000	0.0000	264.7768
1514.0181	9155.8752	645.8867	-0.0000	0.0000	-292.0351
842.1369	645.8867	9244.0565	-0.0000	0.0000	-352.4590
0.0000	-0.0000	-0.0000	4842.5445	52.1913	0.0000
0.0000	0.0000	0.0000	52.1913	4279.2063	-0.0000
264.7768	-292.0351	-352.4590	0.0000	0.0000	4506.8976

[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].