SACADA Database Code: 402

Topology: 4^5T54

# of independent nodes (IN): 5
Transitivity: [5896]
Space Group: Cmmm
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
4^5T54 (SACADA #402)		3.369		0.816	387.5	388.2	69.8	SACADA[1]
G93								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

10084.3702	1085.2420	531.2712	0.0000	-0.0000	-0.0115
1085.2420	10714.7278	251.8412	0.0000	-0.0000	-0.0010
531.2712	251.8412	10357.8083	0.0000	0.0000	-0.0117
0.0000	0.0000	0.0000	4345.0871	-0.0060	-0.0000
-0.0000	-0.0000	0.0000	-0.0060	3638.4745	0.0000
-0.0115	-0.0010	-0.0117	-0.0000	0.0000	2376.6163

[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].