SACADA Database Code: 404

Topology: 4^8T30

# of independent nodes (IN): 8
Transitivity: [8(11)(10)7]
Space Group: Imm2
Pearson: oI28
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
4^8T30 (SACADA #404)		3.438		0.736	405.5	457.8	85.9	SACADA[1]
G95								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

10897.1917	387.1550	944.5357	3.0502	0.0634	0.5002
387.1550	10450.1911	753.2752	2.9328	1.9770	0.3836
944.5357	753.2752	11008.2035	7.5527	-0.8417	0.6124
3.0502	2.9328	7.5527	3891.1393	0.7892	-0.8535
0.0634	1.9770	-0.8417	0.7892	3950.1077	0.9501
0.5002	0.3836	0.6124	-0.8535	0.9501	5150.8819

[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].