SACADA Database Code: 394

Topology: 4^8T25

# of independent nodes (IN): 8
Transitivity: [8(18)(15)6]
Space Group: P-1
Pearson: aP16
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
4^8T25 (SACADA #394)		3.379		0.897	392.7	425.0	78.9	SACADA[1]
G85								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

8619.0957	926.1545	1729.2971	412.6601	100.6216	20.7094
926.1545	10320.1174	927.3214	949.8616	-174.7645	87.5873
1729.2971	927.3214	9278.0980	-428.8793	-230.1445	-127.5969
412.6601	949.8616	-428.8793	4261.9201	190.5521	-85.1844
100.6216	-174.7645	-230.1445	190.5521	4451.1991	276.1211
20.7094	87.5873	-127.5969	-85.1844	276.1211	4420.7348

[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].