SACADA Database Code: 298

Topology: 4^8T19

# of independent nodes (IN): 8
Transitivity: [8(16)(15)6]
Space Group: P21/c
Pearson: mP32
Coordination Number (CN): 4

Year: 2016

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^8T19 (SACADA #298)		3.590		0.814	384.2	489.9	93.5	SACADA[1]
m32		3.524	5.19		345			doi: 10.1103/PhysRevB.94.174102

Elasticity tensor (kBar)[1]

11080.1691	353.6155	375.8356	-0.0000	-0.0000	68.7235
353.6155	10093.1985	465.7500	-0.0000	-0.0000	-158.1523
375.8356	465.7500	11047.0054	-0.0000	0.0000	34.0307
-0.0000	-0.0000	-0.0000	4688.1603	-147.9891	-0.0000
-0.0000	-0.0000	0.0000	-147.9891	4706.8846	0.0000
68.7235	-158.1523	34.0307	-0.0000	0.0000	4790.5495

[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].