SACADA Database Code: 422

Topology: 4^8T32

# of independent nodes (IN): 8
Transitivity: [8(19)(18)9]
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
4^8T32 (SACADA #422)		3.402		1.044	380.8	419.5	78.3	SACADA[1]
G122								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

8593.8231	1338.5178	1021.6786	84.5259	-133.3813	404.1042
1338.5178	9655.1402	829.5321	-350.5258	496.3938	-59.3789
1021.6786	829.5321	9688.4941	115.2725	96.7674	-536.3631
84.5259	-350.5258	115.2725	4134.9443	-300.2943	219.3040
-133.3813	496.3938	96.7674	-300.2943	4505.8408	30.5202
404.1042	-59.3789	-536.3631	219.3040	30.5202	4158.8704

[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].