SACADA Database Code: 319

Topology: 4^{10}T6

# of independent nodes (IN): 10
Transitivity: [(10)(21)(14)3]
Space Group: P-1
Pearson: aP20
Coordination Number (CN): 4

Year: 2013

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^{10}T6 (SACADA #319)		3.226		1.235	327.4	334.1	60.6	SACADA[1]
phaseIII	290	3.16	5.1		427			doi: 10.1016/j.carbon.2013.06.086

Elasticity tensor (kBar)[1]

8096.2111	1369.7671	612.0228	412.6526	61.8336	195.5303
1369.7671	7418.0817	897.0929	173.8689	-128.7030	138.0880
612.0228	897.0929	8199.0404	-200.0713	236.0613	-41.3681
412.6526	173.8689	-200.0713	3536.6721	275.3005	-212.3468
61.8336	-128.7030	236.0613	275.3005	3181.0283	176.7057
195.5303	138.0880	-41.3681	-212.3468	176.7057	3121.2172

[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].