

SACADA Database Code: 83

Topology: [umq](#) 

of independent nodes (IN): 1
Transitivity: [1452]
Space Group: I4/mcm
Pearson: tI32
Coordination Number (CN): 4

Year: 2011

Data

Name	Pressure, GPa	Density, g/cm ³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
umq (SACADA #83)		3.019		0.471	360.0	301.1	45.4	SACADA ¹
TA5								doi: 10.1134/s1063776111060173 
TA5								link 

Elasticity tensor (kBar)¹

8445.8998	1224.7332	1128.6344	0.0000	0.0000	0.0000
1224.7332	8445.8998	1128.6344	0.0000	-0.0000	0.0000
1128.6344	1128.6344	8544.4050	-0.0000	-0.0000	-0.0000
-0.0000	-0.0000	-0.0000	1672.0136	-0.0000	-0.0000
0.0000	-0.0000	0.0000	-0.0000	3369.8136	-0.0000
0.0000	0.0000	-0.0000	0.0000	-0.0000	3369.8136

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 $2\pi \times 0.025 \text{ \AA}^{-1}$ 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 $\text{\AA}^{-1}$ 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].

