

SACADA Database Code: 211

Topology: [cla](#) 

of independent nodes (IN): 4
Transitivity: [4652]
Space Group: I-43m
Pearson: cI82
Coordination Number (CN): 4

Year: 2013

Data

Name	Pressure, GPa	Density, g/cm ³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
cla (SACADA #211)		3.039		0.796	370.1	395.9	73.2	SACADA ¹
KIV		3.01	4.08		354.2		81.7	doi: 10.1063/1.4802002 

Elasticity tensor (kBar)¹

9050.2327	1026.3606	1026.3606	0.0000	0.0000	-0.0000
1026.3606	9050.2327	1026.3606	-0.0000	0.0000	0.0000
1026.3606	1026.3606	9050.2327	0.0000	0.0000	-0.0000
-0.0000	-0.0000	0.0000	3922.7397	0.0000	-0.0000
0.0000	-0.0000	0.0000	0.0000	3922.7397	-0.0000
0.0000	0.0000	-0.0000	-0.0000	-0.0000	3922.7397

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 $10^{-5} \text{ eV \AA}^{-1}$ 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].