SACADA Database Code: 51

Topology: uoc

# of independent nodes (IN): 1
Transitivity: [1231]
Space Group: I4122
Pearson: tI8
Coordination Number (CN): 4

Year: 2004

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
uoc (SACADA #51)		3.246		2.235	291.8	189.7	21.6	SACADA[1]
K		3.176	Metal		333.2			doi: 10.1103/PhysRevB.70.045101

Elasticity tensor (kBar)[1]

7859.0750	3009.4095	2990.1092	0.0000	0.0000	0.0000
3009.4095	3511.9769	1574.2094	0.0000	-0.0000	-0.0000
2990.1092	1574.2094	3520.5416	0.0000	-0.0000	-0.0000
-0.0000	-0.0000	0.0000	3105.0851	0.0000	-0.0000
0.0000	-0.0000	-0.0000	0.0000	2113.5299	0.0000
0.0000	-0.0000	-0.0000	-0.0000	0.0000	3126.0433

[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].