SACADA Database Code: 124

Topology: bik

# of independent nodes (IN): 2
Transitivity: [2432]
Space Group: Cmcm
Pearson: oS12
Coordination Number (CN): 4

Year: 1993

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
bik (SACADA #124)		3.278		0.797	397.9	444.5	83.2	SACADA[1]
C-BIK			3.14					doi: 10.1002/anie.199307011

Elasticity tensor (kBar)[1]

12263.0549	769.8951	57.1004	0.0000	-0.0000	-0.0000
769.8951	8919.1161	1082.2700	0.0000	-0.0000	-0.0000
57.1004	1082.2700	10957.0091	0.0000	0.0000	-0.0000
0.0000	0.0000	0.0000	3428.8600	-0.0000	-0.0000
-0.0000	-0.0000	0.0000	-0.0000	4872.0354	0.0000
-0.0000	-0.0000	-0.0000	-0.0000	-0.0000	4206.5557

[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].