SACADA Database Code: 370

Topology: bcq

# of independent nodes (IN): 2
Transitivity: [2442]
Space Group: Fmmm
Pearson: oF24
Coordination Number (CN): 4

Year: 2017

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
bcq (SACADA #370)		3.296		0.901	383.5	402.8	74.0	SACADA[1]
G28								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

10605.6918	190.4052	784.5065	-0.0000	-0.0000	-0.0000
190.4052	9333.2384	2670.7367	-0.0000	-0.0000	-0.0000
784.5065	2670.7367	7373.6718	0.0000	0.0000	0.0000
-0.0000	-0.0000	0.0000	3782.6566	0.0000	-0.0000
-0.0000	-0.0000	0.0000	0.0000	5053.8499	0.0000
-0.0000	-0.0000	0.0000	-0.0000	0.0000	3946.5036

[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].