SACADA Database Code: 447

Topology: cfe

# of independent nodes (IN): 3
Transitivity: [3443]
Space Group: R-3m
Pearson: hR18
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
cfe (SACADA #447)		3.545		0.579	450.1	531.8	100.7	SACADA[1]
G153								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

12045.6867	1067.8323	321.4576	0.2052	179.0637	2.0258
1067.8323	12047.2056	319.4254	1.2509	-180.0046	-0.6167
321.4576	319.4254	13002.1429	-1.7947	0.7022	0.3707
0.2052	1.2509	-1.7947	5484.9784	-1.0117	180.2015
179.0637	-180.0046	0.7022	-1.0117	4735.6309	2.6707
2.0258	-0.6167	0.3707	180.2015	2.6707	4739.8523

[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].