SACADA Database Code: 143

Topology: atv

# of independent nodes (IN): 2
Transitivity: [2685]
Space Group: Cmmm
Pearson: oS24
Coordination Number (CN): 4

Year: 2016

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
G232atv (SACADA #143)		3.312		0.281	400.7	399.9	71.7	SACADA[1]
C_{ATV}		3.31	3.10		390.8		90.3	doi: 10.1063/1.4965721
								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

10093.7157	204.9125	2223.1846	-0.0000	0.0000	-0.0000
204.9125	12641.0816	129.4228	-0.0000	-0.0000	0.0000
2223.1846	129.4228	8386.2690	0.0000	-0.0000	0.0000
0.0000	0.0000	0.0000	4149.2891	-0.0000	0.0000
0.0000	-0.0000	-0.0000	-0.0000	3763.0717	0.0000
-0.0000	0.0000	0.0000	0.0000	0.0000	3094.2051

[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].