SACADA Database Code: 437

Topology: 4^4T118

# of independent nodes (IN): 4
Transitivity: [4(10)94]
Space Group: C2/m
Pearson: mS24
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
4^4T118 (SACADA #437)		3.471		0.928	389.7	439.4	82.5	SACADA[1]
G137								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

11300.2800	396.0442	835.3061	-0.0000	-0.0000	214.6793
396.0442	9336.4098	1326.5851	-0.0000	-0.0000	-537.4711
835.3061	1326.5851	9375.9582	-0.0000	-0.0000	434.3591
0.0000	-0.0000	-0.0000	3981.9014	-375.9056	-0.0000
-0.0000	-0.0000	-0.0000	-375.9056	3991.6161	-0.0000
214.6793	-537.4711	434.3591	-0.0000	-0.0000	5004.4410

[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].