SACADA Database Code: 435

Topology: 4^8T39

# of independent nodes (IN): 8
Transitivity: [8(13)(13)7]
Space Group: C2/m
Pearson: mS32
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
4^8T39 (SACADA #435)		3.395		0.760	389.5	441.1	82.9	SACADA[1]
G135								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

9674.0665	844.0864	1072.5781	0.0000	-0.0000	427.1646
844.0864	10864.0795	539.3752	0.0000	-0.0000	-225.2342
1072.5781	539.3752	9631.0212	-0.0000	-0.0000	-396.2077
0.0000	0.0000	-0.0000	4638.2650	-391.3829	0.0000
-0.0000	-0.0000	-0.0000	-391.3829	4382.0379	-0.0000
427.1646	-225.2342	-396.2077	0.0000	-0.0000	3875.3712

[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].