SACADA Database Code: 346

Topology: 4^{20}T1

# of independent nodes (IN): 20
Transitivity: [(20)(30)(27)(17)]
Space Group: Cm
Pearson: mS40
Coordination Number (CN): 4

Year: 2013

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^{20}T1 (SACADA #346)		3.404		0.757	390.3	439.8	82.5	SACADA[1]
Cm-40	23.2	3.353						doi: 10.1063/1.4794424

Elasticity tensor (kBar)[1]

8980.7458	868.8169	1268.9016	-0.0000	0.0000	-367.8247
868.8169	10958.6099	594.1120	-0.0000	-0.0000	-300.1997
1268.9016	594.1120	9767.2509	0.0000	-0.0000	121.8374
-0.0000	-0.0000	0.0000	4723.0039	-456.6966	-0.0000
0.0000	-0.0000	-0.0000	-456.6966	4264.3824	-0.0000
-367.8247	-300.1997	121.8374	-0.0000	-0.0000	4090.5472

[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].