SACADA Database Code: 234

Topology: 4^4T37

# of independent nodes (IN): 4
Transitivity: [4(12)(12)6]
Space Group: C2/m
Pearson: mS32
Coordination Number (CN): 4

Year: 2011

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^4T37 (SACADA #234)		3.337		0.806	406.0	428.8	78.9	SACADA[1]
mC32			3.47		384.5		70.2	doi: 10.1103/PhysRevB.84.161411
mC32								doi: 10.1038/srep00471

Elasticity tensor (kBar)[1]

10186.7628	402.5037	1701.3270	-0.0000	0.0000	226.1383
402.5037	10867.8740	768.5112	-0.0000	-0.0000	-205.3113
1701.3270	768.5112	9742.5310	0.0000	-0.0000	489.1045
-0.0000	0.0000	0.0000	3897.8331	473.5025	-0.0000
0.0000	-0.0000	-0.0000	473.5025	3696.5061	0.0000
226.1383	-205.3113	489.1045	-0.0000	0.0000	4703.4266

[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].