SACADA Database Code: 171

Topology: 3^2,4T216

# of independent nodes (IN): 3
Transitivity: [3542]
Space Group: I41/amd
Pearson: tI64
Coordination Number (CN): 3, 4 (1:1)

Year: 2016

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
3^2,4T216 (SACADA #171)		2.598		0.348	275.2	207.1	26.5	SACADA[1]
C64		2.562	1.32		264	217		doi: 10.1007/s10853-016-0564-6

Elasticity tensor (kBar)[1]

6001.8980	485.6293	1262.6134	-0.0000	-0.0000	-0.0000
485.6293	6001.8980	1262.6134	-0.0000	-0.0000	0.0000
1262.6134	1262.6134	6939.1798	0.0000	0.0000	-0.0000
-0.0000	-0.0000	0.0000	1037.9479	0.0000	0.0000
-0.0000	-0.0000	0.0000	-0.0000	2337.0856	0.0000
-0.0000	0.0000	-0.0000	0.0000	0.0000	2337.0857

[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].