SACADA Database Code: 259

Topology: 4^6T6

# of independent nodes (IN): 6
Transitivity: [6996]
Space Group: Amm2
Pearson: oS20
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
4^6T6 (SACADA #259)		3.352		0.757	408.8	445.7	82.9	SACADA[1]
Amm2	24.5	3.303					84.0	doi: 10.1063/1.4794424
Amm2								doi: 10.1209/0295-5075/108/46006

Elasticity tensor (kBar)[1]

11400.3922	407.1359	902.5437	0.0000	0.0000	0.0000
407.1359	11783.2348	1084.0371	-0.0000	-0.0000	0.0000
902.5437	1084.0371	8983.6914	0.0000	-0.0000	0.0000
0.0000	-0.0000	0.0000	4649.9752	-0.0000	0.0000
0.0000	-0.0000	-0.0000	-0.0000	3768.0927	-0.0000
0.0000	0.0000	0.0000	0.0000	-0.0000	4158.0601

[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].