SACADA Database Code: 240

Topology: 4^5T29

# of independent nodes (IN): 5
Transitivity: [5765]
Space Group: R32
Pearson: hR45
Coordination Number (CN): 4

Year: 2015

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^5T29 (SACADA #240)		3.369		0.736	408.6	450.2	84.0	SACADA[1]
HR-carbon	14.2		4.6		427		80	doi: 10.1038/srep13447

Elasticity tensor (kBar)[1]

10038.4509	811.8590	777.9200	-0.0000	42.7624	0.0000
811.8590	10038.4509	777.9200	-0.0000	-42.7624	0.0000
777.9200	777.9200	12095.7617	0.0000	0.0000	-0.0000
-0.0000	-0.0000	0.0000	4613.2960	0.0000	42.7624
42.7624	-42.7624	0.0000	0.0000	4045.9140	0.0000
0.0000	0.0000	-0.0000	42.7624	-0.0000	4045.9140

[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].