SACADA Database Code: 30

Topology: neb

# of independent nodes (IN): 1
Transitivity: [1221]
Space Group: Fddd
Pearson: oF16
Coordination Number (CN): 4

Year: 2004

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
neb (SACADA #30)		3.581		1.675	380.6	415.1	77.2	SACADA[1]
H-carbon		3.532						doi: 10.1103/PhysRevB.70.045101
								doi: 10.1524/zkri.2013.1620

Elasticity tensor (kBar)[1]

14197.9686	60.6343	510.0209	-0.0000	-0.0000	0.0000
60.6343	7823.6833	650.0310	-0.0000	-0.0000	0.0000
510.0209	650.0310	10730.2718	-0.0000	-0.0000	0.0000
-0.0000	-0.0000	-0.0000	3665.3101	-0.0000	0.0000
-0.0000	-0.0000	-0.0000	-0.0000	2628.5076	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	4908.9694

[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].