SACADA Database Code: 498

Topology: 4^8T48

# of independent nodes (IN): 8
Transitivity: [8(18)(12)2]
Space Group: C2
Pearson: mS32
Coordination Number (CN): 4

Year: 2017

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^8T48 (SACADA #498)		3.367		0.806	397.7	432.0	80.3	SACADA[1]
G210								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

9688.1383	833.6318	836.9416	-0.0001	-0.0000	13.9194
833.6318	9760.6990	1127.6037	-0.0001	-0.0000	-81.6657
836.9416	1127.6037	10800.6983	-0.0000	-0.0000	-49.0284
-0.0001	-0.0001	-0.0000	3475.0835	-79.1095	-0.0000
-0.0000	-0.0000	-0.0000	-79.1095	4919.2814	-0.0001
13.9194	-81.6657	-49.0284	-0.0000	-0.0001	4223.2057

[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].