SACADA Database Code: 628

Topology: umq

# of independent nodes (IN): 1
Transitivity: [1452]
Space Group: I4/mcm
Pearson: tI32
Coordination Number (CN): 4

Year: 2021

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
umq (SACADA #628)		3.019		0.471	359.8	299.6	44.8	SACADA[1]
umq								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

8426.8969	1221.8447	1134.6383	0.0000	0.0000	0.0000
1221.8447	8426.8969	1134.6383	-0.0000	0.0000	-0.0000
1134.6383	1134.6383	8542.2527	-0.0000	-0.0000	-0.0000
-0.0000	-0.0000	-0.0000	1652.3758	-0.0000	-0.0000
0.0000	0.0000	0.0000	-0.0000	3357.5781	0.0000
0.0000	0.0000	-0.0000	-0.0000	-0.0000	3357.5781

[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].