MATERIAL DATA SHEET

Calcium carbonate, calcite structure (CaCO3)

Open JARVIS-DFT screening card for CaCO3: density, elastic moduli, structure, and selected calculated electronic/energy fields.

Field	Value
Material ID	jarvis-jvasp-9573
Category	Glass / Ceramic
Condition	ideal computational crystal | periodic bulk crystal model
Unit system	Common SI
Unit contract	Material properties stored in SI engineering units.
Generated	2026-11-15 23:19

Source and Validity

Field	Value
Quality	Computational screening
Design release allowed	No
Source family	Computational dataset
Confidence	Engineering estimate
License	Open
Source note	CC BY 4.0 JARVIS-DFT computational crystal record generated from a pinned, hash-checked source subset.
Citation	JARVIS-DFT 3D dataset, Figshare article version 11, record JVASP-9573, DOI 10.6084/m9.figshare.6815699.v11, CC BY 4.0; https://jarvis.nist.gov/
Valid temperature	0 ... 0 K (Static DFT equilibrium-crystal screening condition; finite-temperature behavior is not modeled.)
Valid pressure	Relaxed computational structure; no engineering pressure-validity range is established.
Valid phase / condition	JARVIS-DFT ideal trigonal crystal, space group R-3c (No. 167), static relaxed structure.
Uncertainty	Computational screening values, not measured material-card values. Verify phase, composition, porosity, defects, temperature, processing, and product form.
Last reviewed	2026-07-30
Reviewer	scripts/import_jarvis_public_solids.py
Review status	Checked
Review scope	Checked pinned hashes, CC BY attribution, selected JARVIS identities, units, and deterministic conversions; not validated for engineering release.
Notes	Ideal computational phase; not a manufacturer grade or design allowable.
License ID	CC-BY-4.0

Field	Value
License URL	https://creativecommons.org/licenses/by/4.0/
Attribution	Kamal Choudhary and the NIST JARVIS team

Material Condition

Field	Value
Condition	ideal computational crystal
Product form	periodic bulk crystal model
Thickness / diameter range	Not applicable to the computational unit cell.
Test direction	Voigt isotropic elastic average.
Processing route	Static DFT relaxation using the upstream JARVIS workflow.
Temperature range	0 ... 0 K
Notes	Computational screening values, not measured material-card values. Verify phase, composition, porosity, defects, temperature, processing, and product form.

Properties

Physical

Property	Value	Unit	Type	Applies to
Density	2687	kg/m^3	Computed	JARVIS-DFT ideal trigonal crystal, space group R-3c (No. 167), static relaxed structure.

Mechanical

Property	Value	Unit	Type	Applies to
Bulk modulus	86.91	GPa	Computed	JARVIS-DFT ideal trigonal crystal, space group R-3c (No. 167), static relaxed structure. Voigt elastic average.
Shear modulus	38.53	GPa	Computed	JARVIS-DFT ideal trigonal crystal, space group R-3c (No. 167), static relaxed structure. Voigt elastic average.
Young's modulus	100.70768128049188	GPa	Derived Computed	JARVIS-DFT ideal trigonal crystal, space group R-3c (No. 167), static relaxed structure. Isotropic value derived from the upstream Voigt K and G.
Poisson's ratio	0.32	-	Computed	JARVIS-DFT ideal trigonal crystal, space group R-3c (No. 167), static relaxed structure. Upstream JARVIS value.

Electronic

Property	Value	Unit	Type	Applies to
DFT band gap	5.169	eV	Computed	JARVIS-DFT ideal trigonal crystal, space group R-3c (No. 167), static relaxed structure. OptB88vdW calculation.

Identity

Property	Value	Unit	Type	Applies to
Chemical formula	CaCO3	-	Computed	JARVIS-DFT ideal trigonal crystal, space group R-3c (No. 167), static relaxed structure.

Structure

Property	Value	Unit	Type	Applies to
Crystal system	trigonal	-	Computed	JARVIS-DFT ideal trigonal crystal, space group R-3c (No. 167), static relaxed structure.
Space group	R-3c (No. 167)	-	Computed	JARVIS-DFT ideal trigonal crystal, space group R-3c (No. 167), static relaxed structure.

Thermodynamic

Property	Value	Unit	Type	Applies to
Formation energy per atom	-2.41013	eV/atom	Computed	JARVIS-DFT ideal trigonal crystal, space group R-3c (No. 167), static relaxed structure. Upstream calculated formation energy.

Engineering note: seed solid-material values are reference values only. Verify against the project material specification or supplier data sheet before release.