MATERIAL DATA SHEET

# Barium titanate, tetragonal phase (BaTiO3)

Open JARVIS-DFT screening card for BaTiO3: density, elastic moduli, structure, and selected calculated electronic/energy fields.

| Field | Value |
|---|---|
| Material ID | jarvis-jvasp-110 |
| 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-110, 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 tetragonal crystal, space group P4mm (No. 99), 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 | 5847 | kg/m^3 | Computed | JARVIS-DFT ideal tetragonal crystal, space group P4mm (No. 99), static relaxed structure. |

## Mechanical

| Property | Value | Unit | Type | Applies to |
|---|---|---|---|---|
| Bulk modulus | 139.67 | GPa | Computed | JARVIS-DFT ideal tetragonal crystal, space group P4mm (No. 99), static relaxed structure. Voigt elastic average. |
| Shear modulus | 97.22 | GPa | Computed | JARVIS-DFT ideal tetragonal crystal, space group P4mm (No. 99), static relaxed structure. Voigt elastic average. |
| Young's modulus | 236.73257385274005 | GPa | Derived Computed | JARVIS-DFT ideal tetragonal crystal, space group P4mm (No. 99), static relaxed structure. Isotropic value derived from the upstream Voigt K and G. |
| Poisson's ratio | 0.22 | - | Computed | JARVIS-DFT ideal tetragonal crystal, space group P4mm (No. 99), static relaxed structure. Upstream JARVIS value. |

## Electronic

| Property | Value | Unit | Type | Applies to |
|---|---|---|---|---|
| DFT band gap | 1.749 | eV | Computed | JARVIS-DFT ideal tetragonal crystal, space group P4mm (No. 99), static relaxed structure. OptB88vdW calculation. |

## Identity

| Property | Value | Unit | Type | Applies to |
|---|---|---|---|---|
| Chemical formula | BaTiO3 | - | Computed | JARVIS-DFT ideal tetragonal crystal, space group P4mm (No. 99), static relaxed structure. |

## Structure

| Property | Value | Unit | Type | Applies to |
|---|---|---|---|---|
| Crystal system | tetragonal | - | Computed | JARVIS-DFT ideal tetragonal crystal, space group P4mm (No. 99), static relaxed structure. |
| Space group | P4mm (No. 99) | - | Computed | JARVIS-DFT ideal tetragonal crystal, space group P4mm (No. 99), static relaxed structure. |

## Thermodynamic

| Property | Value | Unit | Type | Applies to |
|---|---|---|---|---|
| Formation energy per atom | -3.35196 | eV/atom | Computed | JARVIS-DFT ideal tetragonal crystal, space group P4mm (No. 99), 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.