

Materials Project **API key** is here

The screenshot shows the Materials Project dashboard in a Chrome browser. The URL bar displays <https://materialsproject.org/dashboard>. The user is logged in as 'metokal@gmail.com'. The dashboard includes a navigation bar with links to Home, About, Apps, Documentation, API, Tutorials, and Dashboard. On the left, there are sections for 'Privileges' (User), 'Default App' (materials explorer), and 'Sandbox DB' (core). A red arrow points from the text 'Materials Project API key is here' to a red dashed circle around the 'Generate API Key' button. Below this, the 'Predicted Structures' section lists two entries: 'Co:[3], O:[-2], La:[3]' (ID: 2256, CREATED June 3, 2013, 12:57 p.m.) and 'Pr:[3], Co:[3], O:[-2]' (ID: 1689, COMPLETED Feb. 5, 2013, 4:16 p.m.). A 'More Details' button is next to the second entry. At the bottom, there is a 'Questions or Feedback?' button.

Materials Project - Google Chrome

Materials Project

Secure | <https://materialsproject.org/dashboard>

Home About Apps Documentation API Tutorials Dashboard

metokal@gmail.com

[Generate API Key](#)

Receive email updates from the Materials Project ☒

Privileges
User

Default App
materials explorer

Sandbox DB
core

Predicted Structures

Co:[3], O:[-2], La:[3] CREATED June 3, 2013, 12:57 p.m.	ID : 2256
Pr:[3], Co:[3], O:[-2] COMPLETED Feb. 5, 2013, 4:16 p.m.	ID : 1689 More Details →

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[Questions or Feedback?](#)

Materials Project *ID (mpid)* is here

mp-5229: SrTiO₃ (cubic, Pm-3m, 221) - Google Chrome

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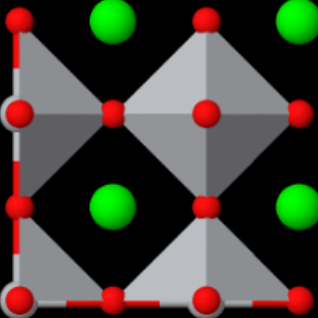
Secure | <https://materialsproject.org/materials/mp-5229/>

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MATERIAL ID: **mp-5229** DOI: 10.17188/1263154 Show Help Guides

X-Ray Diffraction X-Ray Absorption Substrates Elasticity Calculation Summary Provenance/Citation

HM: P 1
a=3.945 Å
b=3.945 Å
c=3.945 Å
α=90.000°
β=90.000°
γ=90.000°



Structure Type: Conventional Standard Primitive Refined CIF

☐ Space Filling ☒ Polyhedra

Zoom in/out Shift + Drag cursor
Rotate along the center axis Option + Drag cursor

Edit Crystal Generate Phase Diagram

Tags: Taosonite Strontium titanate

Material Details

Final Magnetic Moment
0.000 μ_B

Magnetic Ordering
Unknown

Formation Energy / Atom
-3.569 eV

Energy Above Hull / Atom
0.001 eV

Density
4.96 g/cm³

Decomposes To
[SrTiO₃](#)

Band Gap
2.103 eV

Lattice Parameters

computed ICSD

a 3.945 Å α 90.000°
b 3.945 Å β 90.000°
c 3.945 Å γ 90.000°
Volume 61.402 Å³

Final Structure

Fractional Coordinates CIF

O		
a	b	c
0	0.5	0.5
0.5	0	0.5
0.5	0.5	0

Ti		
a	b	c
0.5	0.5	0.5

Sr		
a	b	c
0	0	0

Space Group

Hermann Mauguin
Pm $\bar{3}$ m [221]

Hall
-P 4 2 3

Point Group
m $\bar{3}$ m

```

1 ''' Suppose you have an experimental unknown spectrum and you want to
2 compare it with a spectrum in the database. For this task, you can use
3 compare_my_unknown function as below. First you should place your unknown
4 spectrum into "unknowns" folder as two-column plain text and give it a
5 filename like: unknown.txt. then you should provide mpid of reference '''
6
7 compare_my_unknown(fname='unknown.txt',mpid='mvc-11115',absorbing_atom='Ti')

```

executed in 487ms, finished 16:57:25 2018-02-05

x-shift in eV:

1.5

