

Materials Project **API key** is here

The screenshot shows the Materials Project dashboard in a Chrome browser. The URL is <https://materialsproject.org/dashboard>. The user is logged in as 'metokal@gmail.com'. The 'Generate API Key' button is highlighted with a red dashed circle and a red arrow pointing to it from the text above. The button is labeled 'Generate API Key' and has a red squiggle underneath it. The dashboard also shows a 'Default App' dropdown set to 'materials explorer', a 'Sandbox DB' dropdown set to 'core', and a 'Predicted Structures' section with 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>

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metokal@gmail.com

Privileges User

Default App materials explorer

Sandbox DB core

Generate API Key

Receive email updates from the Materials Project

### Predicted Structures

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

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Questions or Feedback?

Materials Project *ID (mpid)* is here

mp-5229: SrTiO<sub>3</sub> (cubic, Pm-3m, 221) - Google Chrome

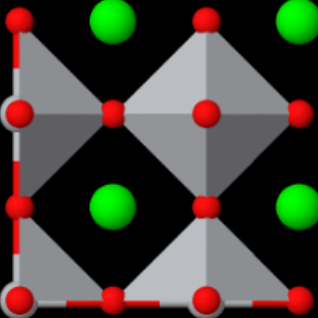
Secure | <https://materialsproject.org/materials/mp-5229/>

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MATERIAL: SrTiO<sub>3</sub> 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:    [CIF](#)

☐ Space Filling ☒ Polyhedra

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

[Edit Crystal](#) [Generate Phase Diagram](#)

Tags: [Tausonite](#) [Strontium titanate](#)

### Material Details

Final Magnetic Moment  
0.000  $\mu_B$

Magnetic Ordering  
Unknown

Formation Energy / Atom  
-3.569 eV

Energy Above Hull / Atom  
0.001 eV

Density  
4.96 g/cm<sup>3</sup>

Decomposes To  
[SrTiO<sub>3</sub>](#)

Band Gap  
2.103 eV [Warning](#)

### 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 Å<sup>3</sup>

### 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