New Materials & Devices

Building Blocks for Future

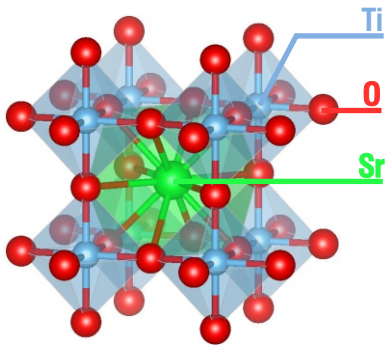
Defect-Induced Eletronic Structure Modification in Co-Doped $SrTiO_3$ Perovskites

Abstract

This study presents the development of $SrTiO_3$ doped with Co^{2+} at the Ti^{4+} site ($SrTi_{1-x}Co_xO_{3-\delta}$), with cobalt atomic concentrations of 0% (undoped), 2,5%, 5% and 10% (x = 0, x=0.025, x = 0.05, 0.10 respectively). With the partial substitution of Ti^{4+} ions by Co^{2+} ions, a charge imbalance occurs that favors the formation and stabilization of oxygen vacancies (V_o), allowing for the restoration of charge neutrality in the structure. The samples were synthesized using the polymeric precursor method (sol-gel/Pechini). The Co-doped $SrTiO_3$ samples were reduced in 500 °C in a controlled atmosphere (Ar + H_2). Structural characterization was performed through thermal analysis, X-ray diffraction, BET and Raman spectroscopy. Diffuse reflectance spectroscopy was used to measure the band-gap energy (E_g) of the samples. The analysis revealed that Co^{2+} substitutes Ti^{4+} in the structure, generating symmetry distortions due to the promotion of V_o. These effects indicate good prospects for catalysis applications, demonstrating that doping is a promising strategy for improving the properties of this material.

Motivation — The Co-Doped Strontium Titanate

Strontium Titanate



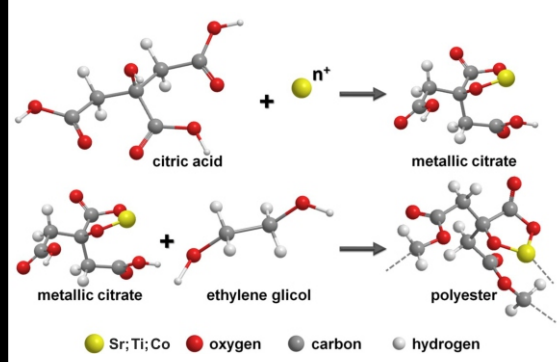
Co-DOPED

- ✓ Oxygen Vacancy
- ✓ Reduced efective band-gap
- ✓ Improved electron-hole pair efficiency
- ✓ Interfacial Polarization

→ **Multifunctionality**
Defect Engineering

Samples — Pechini Method

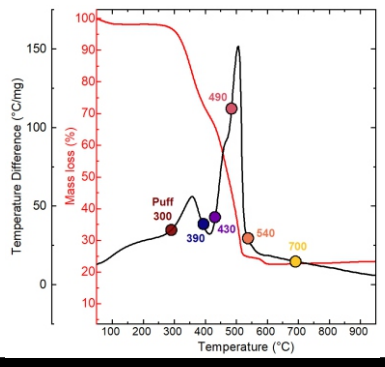
Pechini-Method



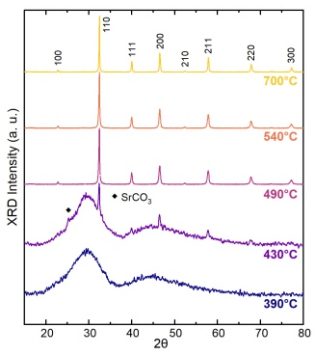
- ✓ STO
- ✓ STOC2.5
- ✓ STOC5
- ✓ STOC10
- ✓ Reduced Samples

Results ❶ Thermal Analysis + XRD

Differential Thermogravimetry

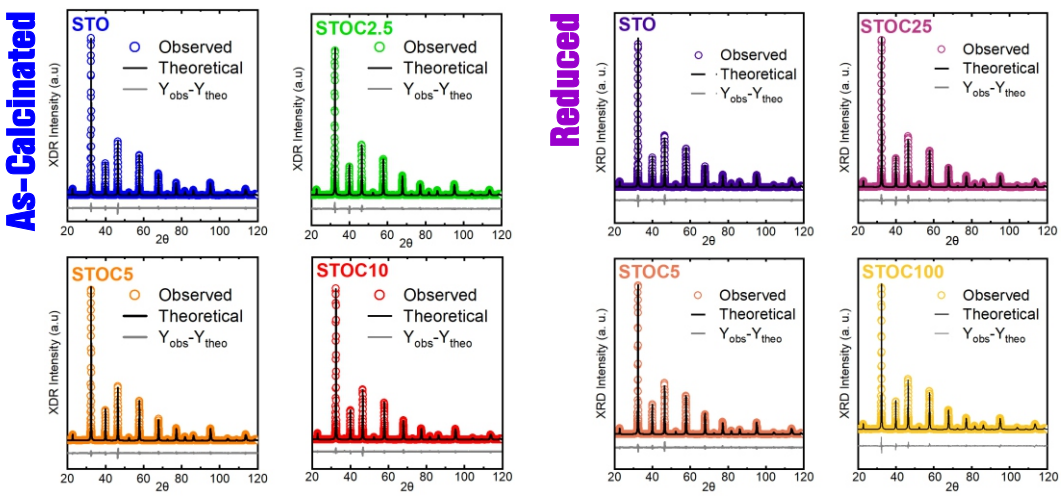


XRD Difraction



- **700 °C**
  Complete organic decomposition.
- **490 °C**
  Pure STO perovskite phase formed.

Results ❷ XRD + Rietveld



Sample	Sr	Ti	O	Co
STO	0.998(5)	1.008(5)	0.996(6)	-
STOC25	0.994(2)	0.976(2)	0.991(3)	0.024(2)
STOC50	0.995(1)	0.952(2)	0.987(3)	0.051(1)
STOC100	0.999(2)	0.898(3)	0.984(4)	0.103(3)

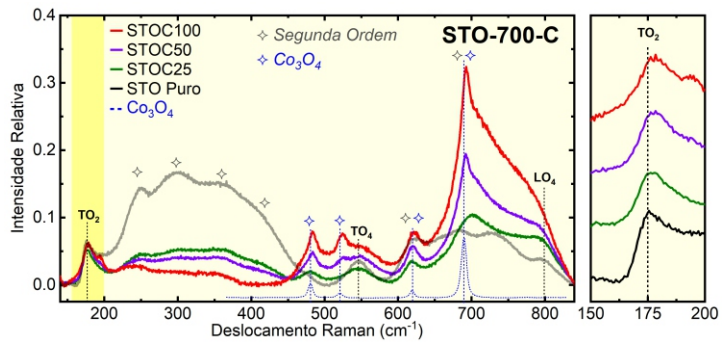
Sample	a (Å)	V (Å³)	χ^2	R_{wp} (%)
STO	3.90832(6)	59.699(3)	2.13	7.98
STOC25	3.90772(2)	59.672(1)	1.80	7.61
STOC50	3.90682(2)	59.631(1)	1.80	7.60
STOC100	3.90566(4)	59.578(2)	1.99	7.88

Sample	Sr	Ti	O	Co
STO	0.994(1)	1.006(2)	0.988(4)	-
STOC25	0.999(1)	0.976(2)	0.977(3)	0.026(2)
STOC50	1.001(1)	0.951(2)	0.967(3)	0.051(1)
STOC100	0.994(2)	0.900(3)	0.954(4)	0.101(3)

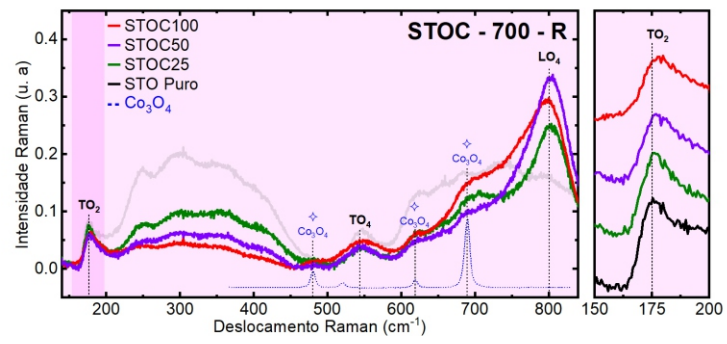
Sample	a (Å)	V (Å³)	χ^2	R_{wp} (%)
STO	3.90832(3)	59.700(1)	2.93	10.33
STOC25	3.90939(2)	59.748(1)	2.23	8.73
STOC50	3.91036(2)	59.793(1)	1.71	7.59
STOC100	3.91213(2)	59.874(2)	1.86	8.25

Results ❸ Vibrational Spectroscopy

As-calcinated (Unreduced)

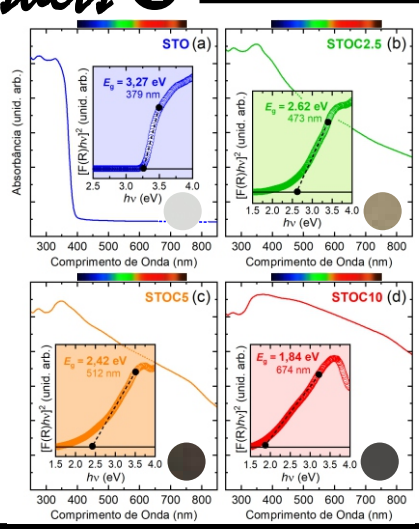


Reduced

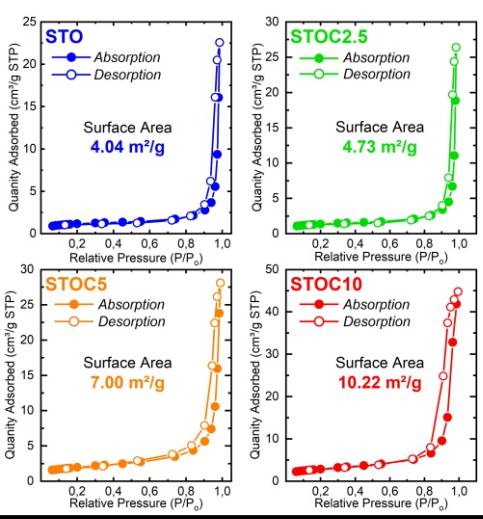


Results ❹ Difuse Photoreflectance + BET

DRS Data



BET Data



Conclusions

The material was successfully synthesized using the polymeric precursor method.

The reduction process successfully introduced oxygen vacancies into the sample.

BET analysis showed that increasing Co content led to smaller grain size and higher surface area.

DRS analysis showed that the band gap decreased with increasing Co concentration, suggesting enhanced photocatalytic potential.

References

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