Innovating Perovskite Materials for High-performing Reversible Solid Oxide Cells

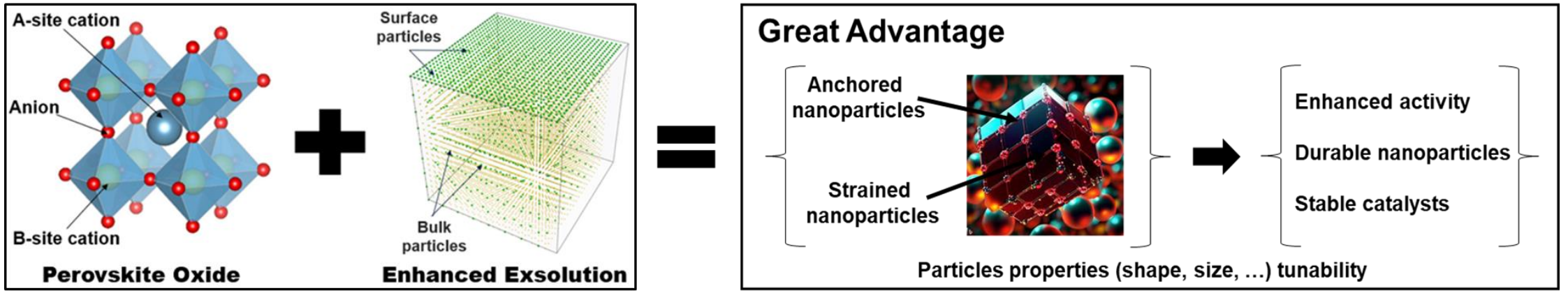
Ubong Essien

Supervisor: Dragos Neagu

12th December 2023

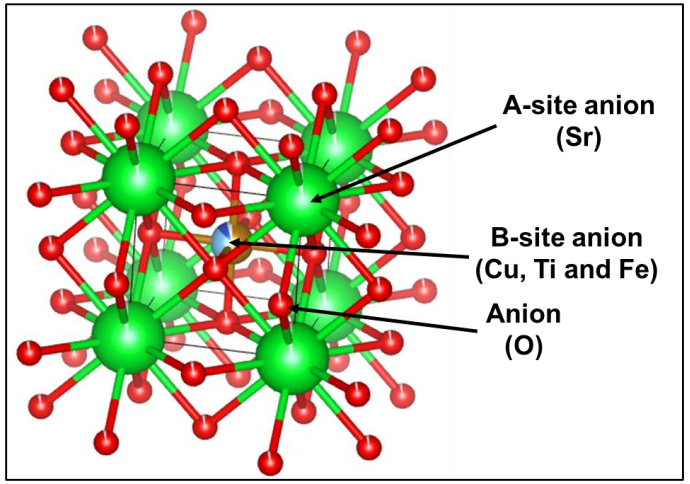
Presentation Outline

Introduction → Research Focus → Materials and Method → Result → Conclusion → Future Work



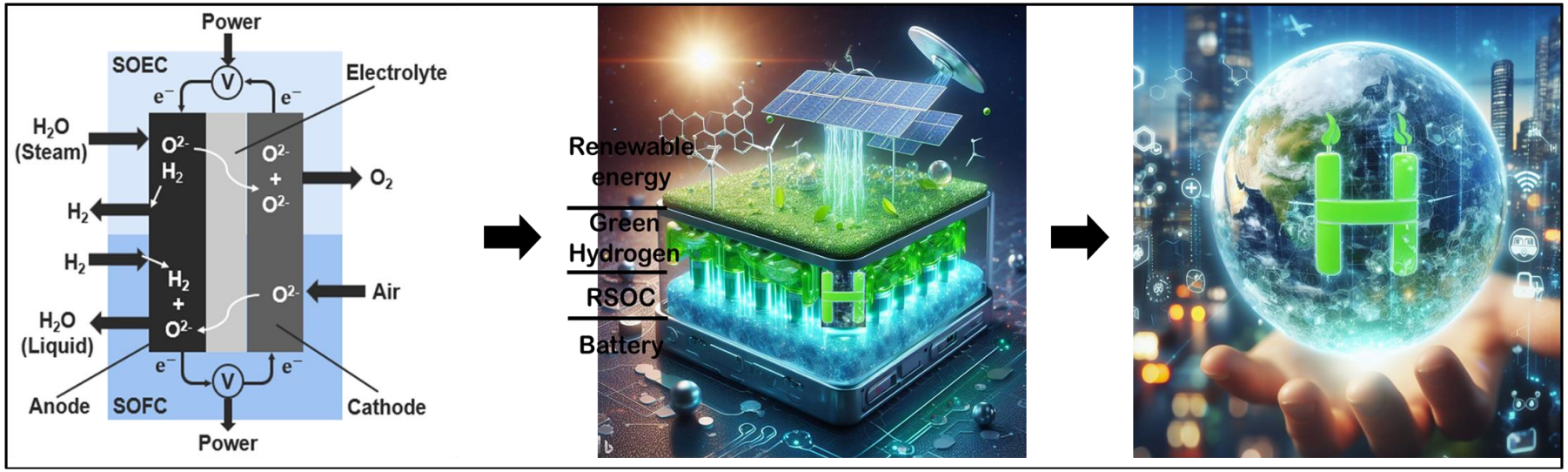
Introduction

❖ **Perovskite oxides, the unique energy materials**



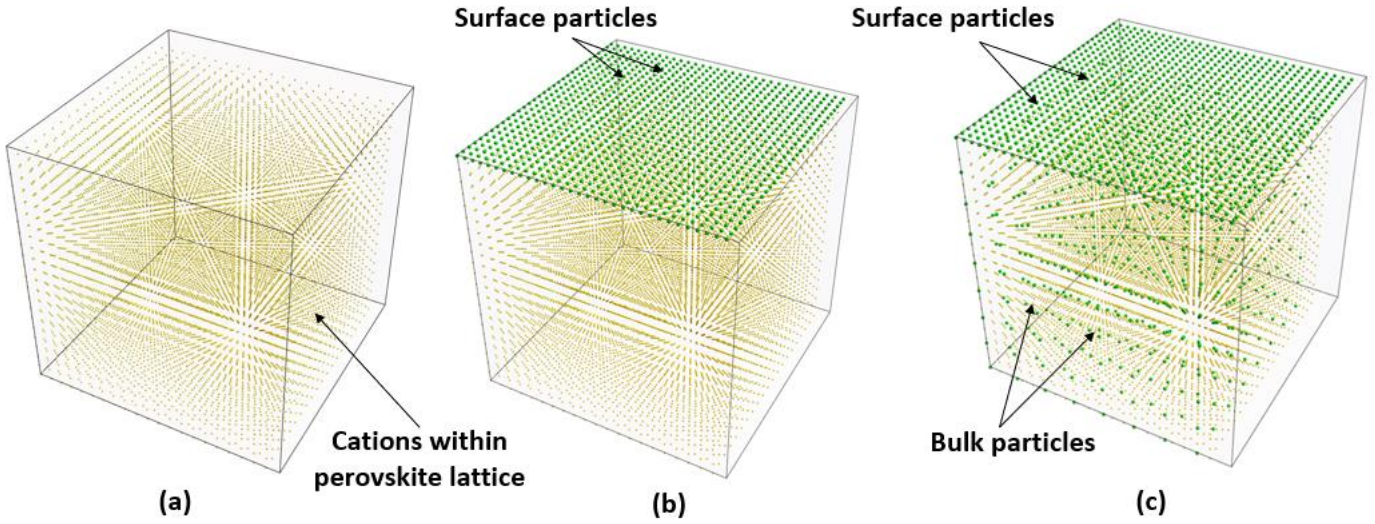
$Sr_{0.95}Ti_{0.3}Fe_{0.6}Cu_{0.1}O_3$
Crystal Structure

- ✓ Versatile and adaptable ABO_3 crystal structure
- ✓ Wide range of chemical substitution
- ✓ Tunable properties: ionic conductivity, electronic conductivity, catalytic activity etc.

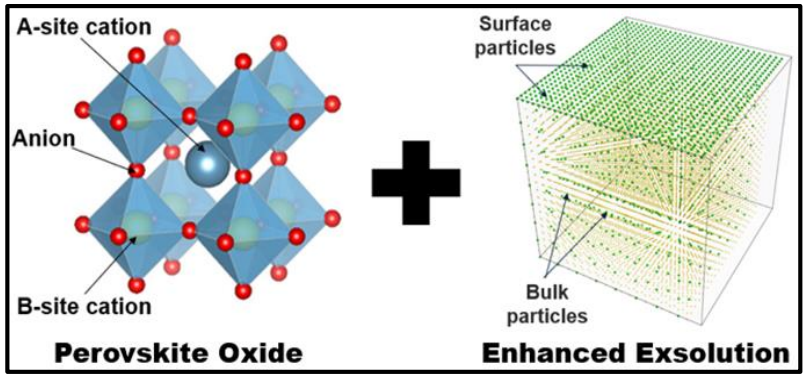


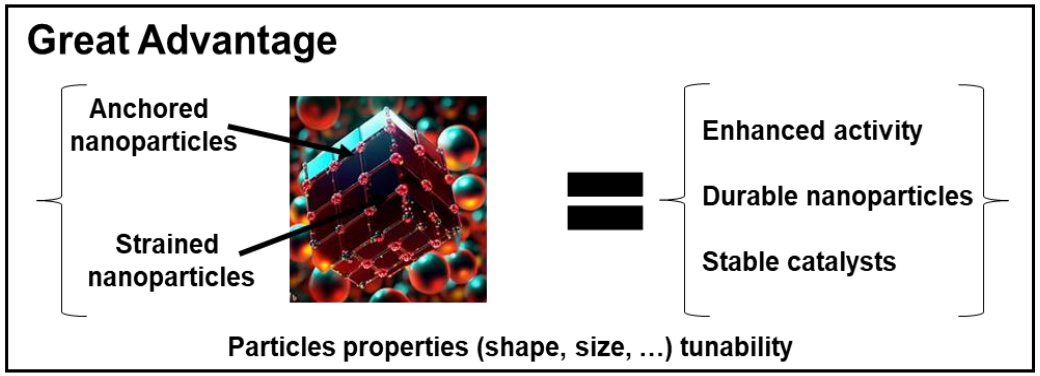
Research Focus

❖ The Need for a Novel Perovskite Material



Schematics of a nanoscale representation of a perovskite lattice at (a) cations segregation, (b) surface exsolution, and (c) bulk and surface exsolution.

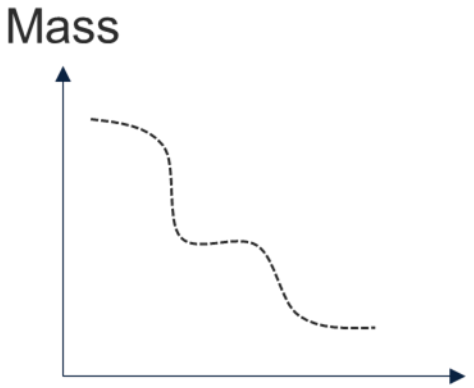


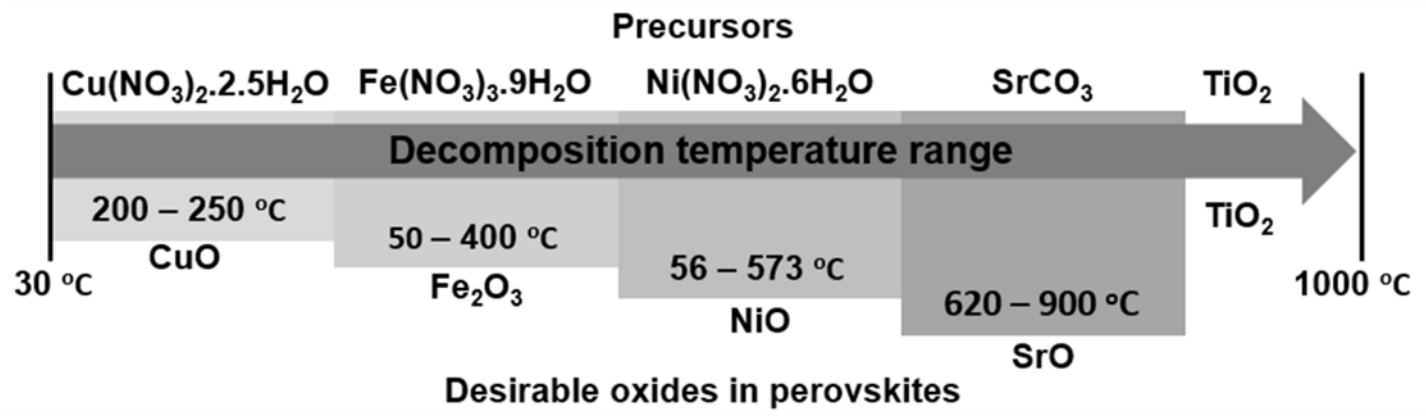


Materials and Method

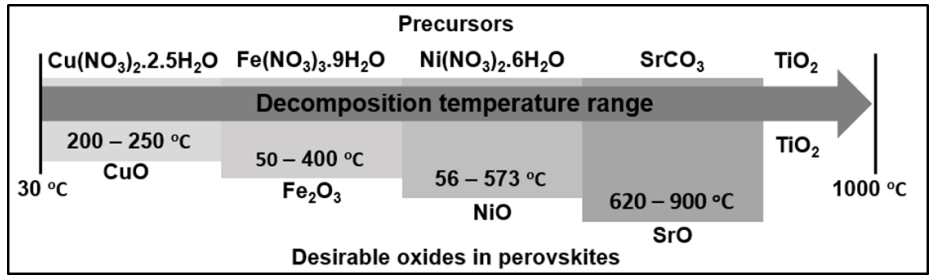
Selected precursors and established synthesis parameters → Synthesized perovskites by solid state method → Characterized the perovskites (TGA, XRD, SEM, etc.) → Reduced the perovskite to study exsolution process

Thermogravimetry analysis (TGA)

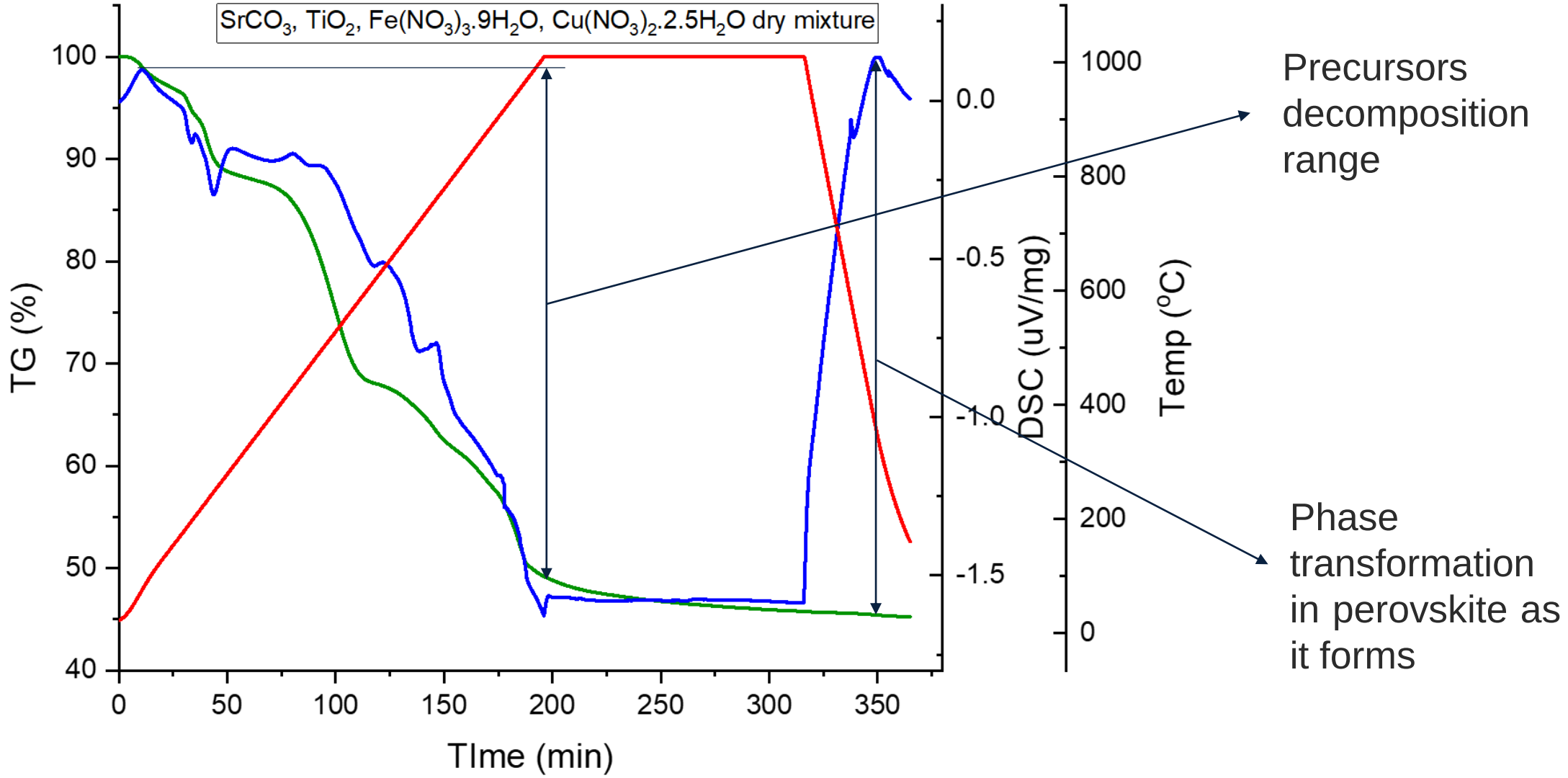




Materials and Method

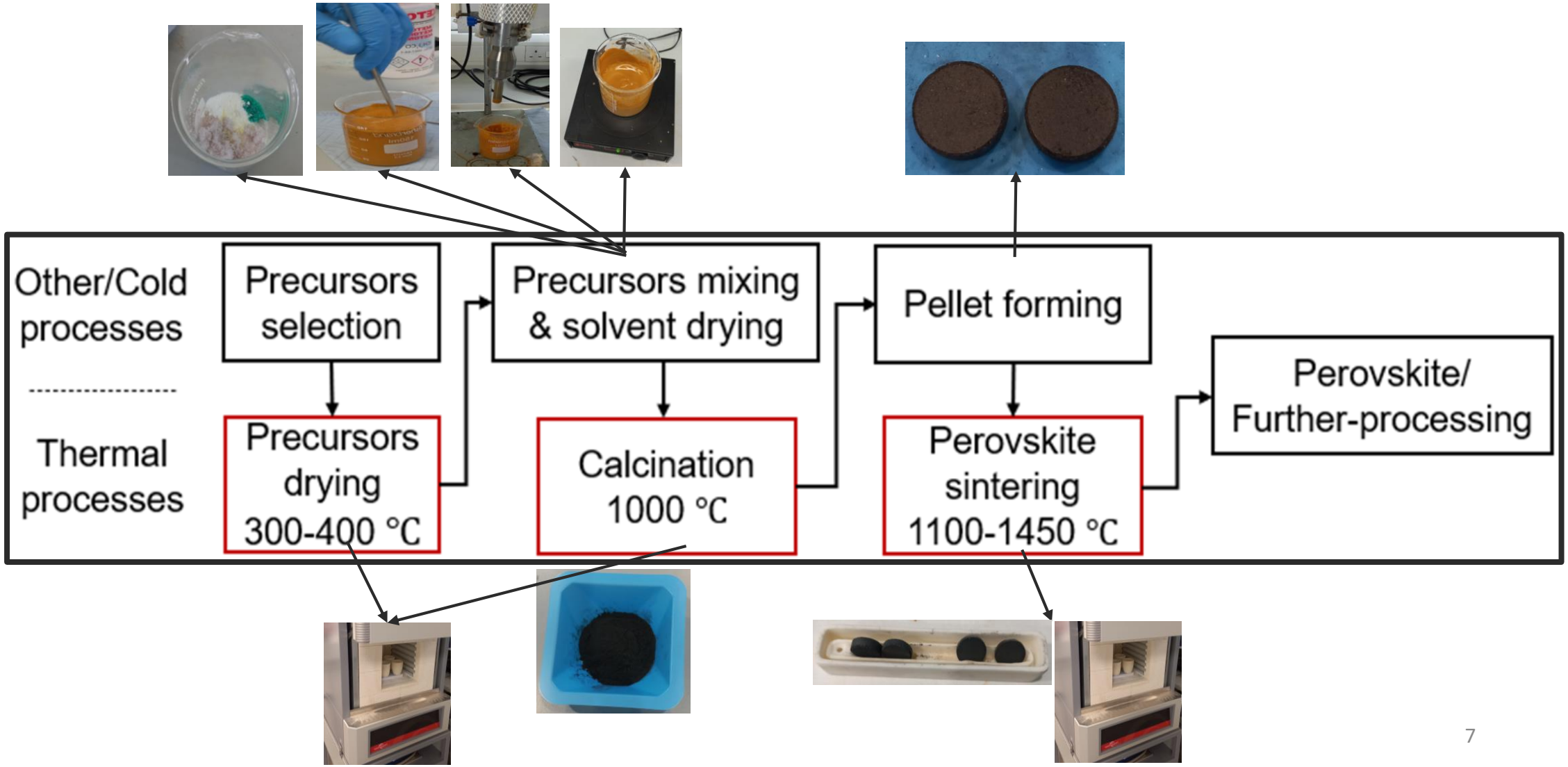


❖ Synthesis parameters prediction



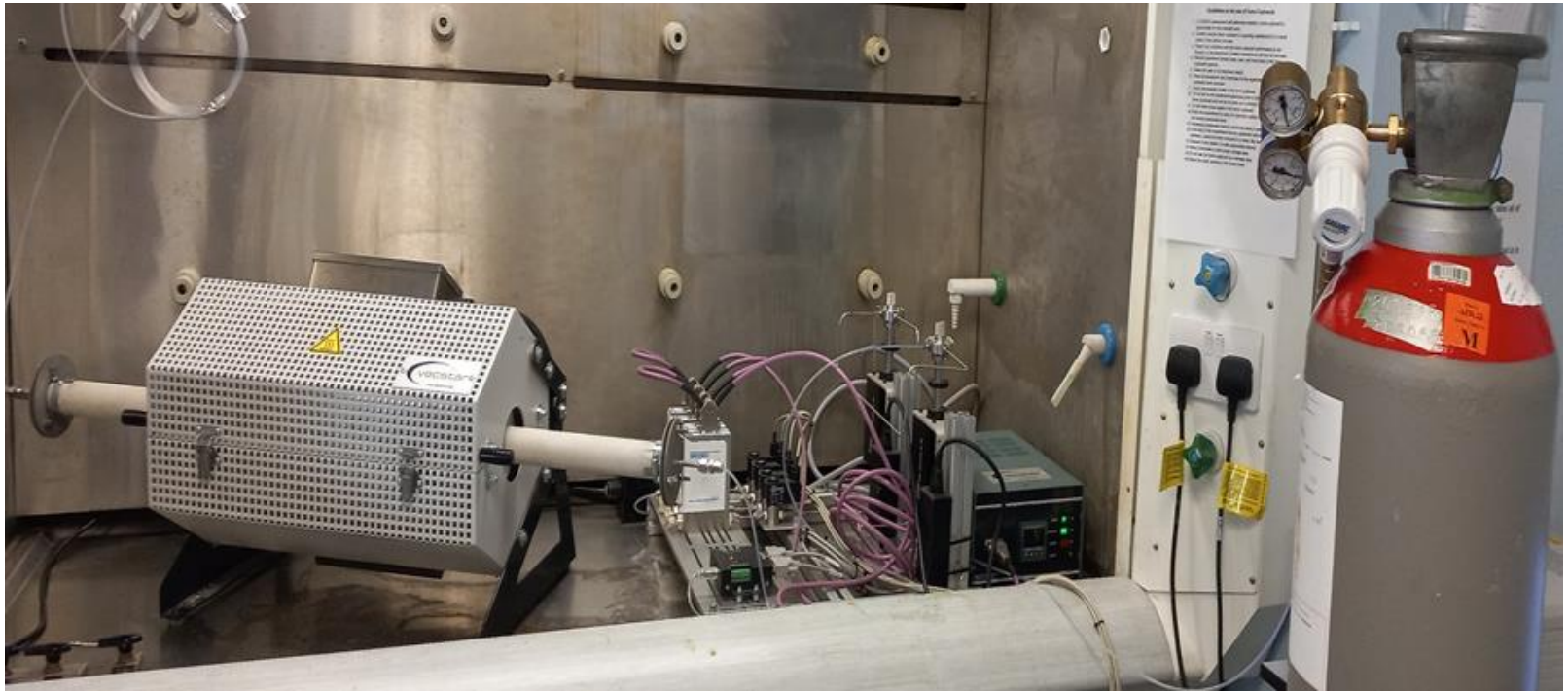
Materials and Method

- **Perovskite synthesis:** solid-state synthesis method



Materials and Method

- **Reduction of the Perovskites in 5 % H_2**

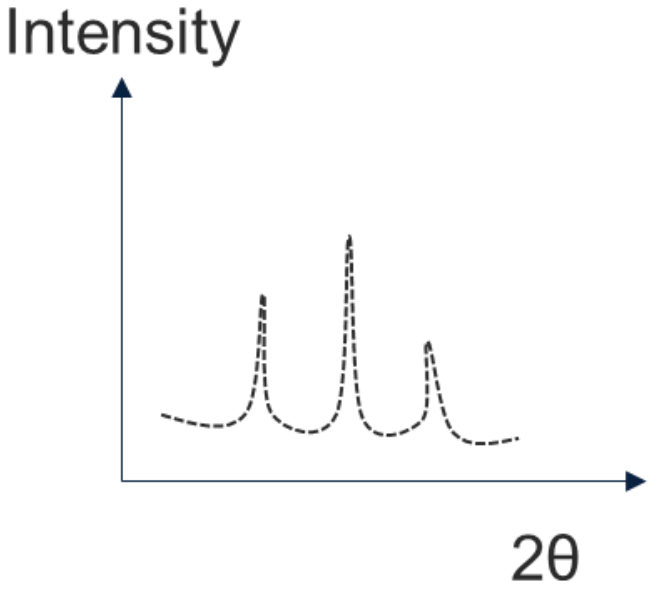


A reduction furnace setup for achieving exsolution in the perovskite after reduction in 5 % H_2

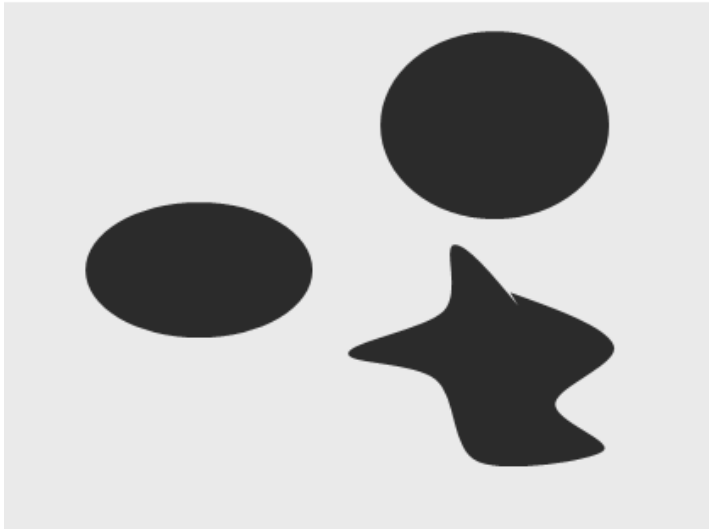
Materials and Method

- **Perovskite Material Characterisation**

X-Ray diffraction analysis (XRD)

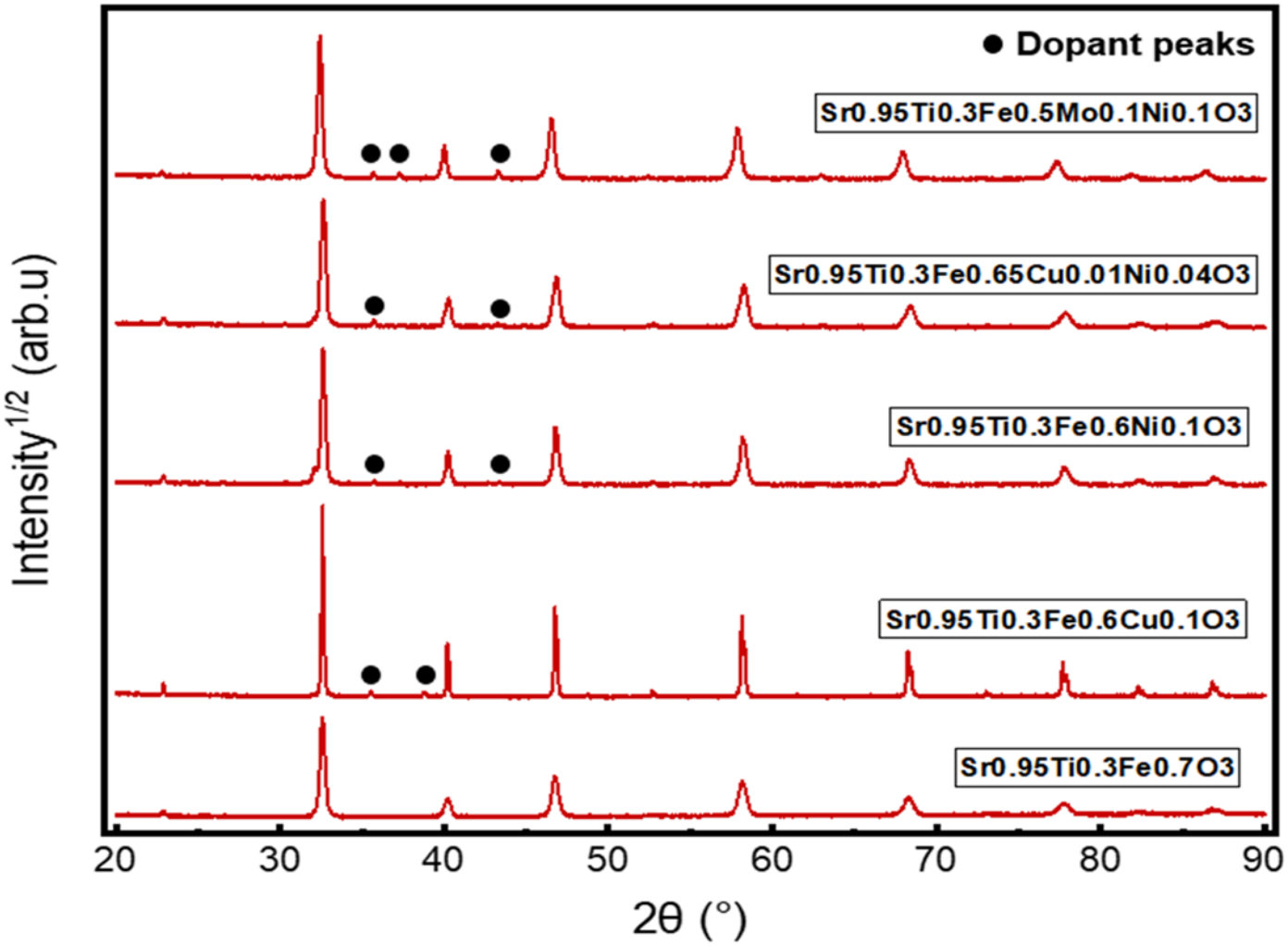


Scanning electron microscopy (SEM)



Result

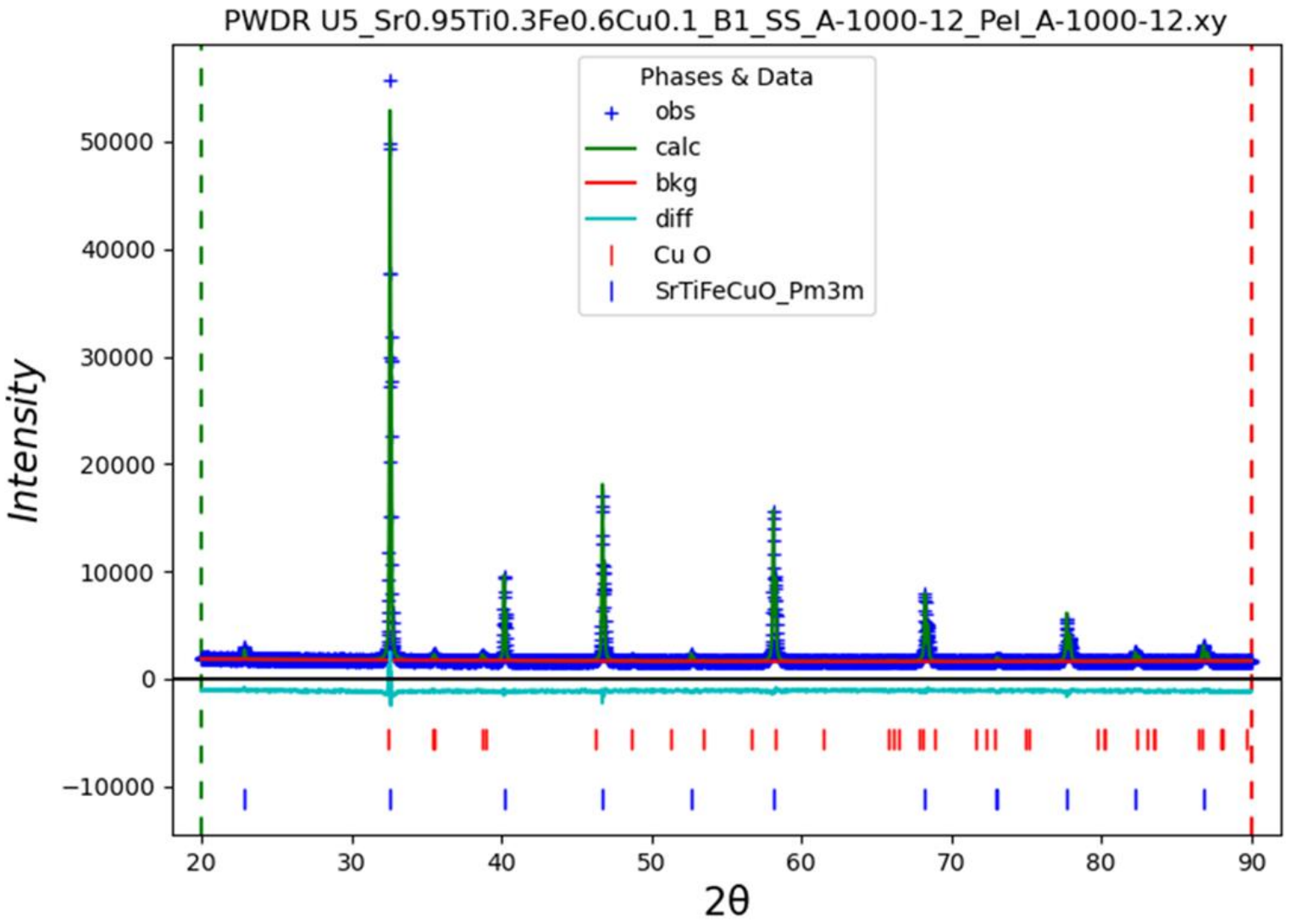
- **XRD result of synthesized perovskites**

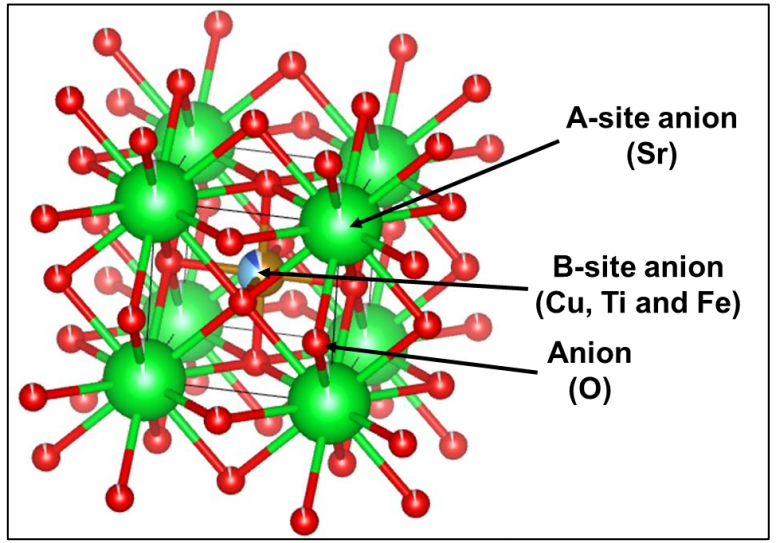


Room temperature powder XRD pattern of four perovskites synthesized from doping **A-site deficient $Sr_{0.95}Ti_{0.3}Fe_{0.7}O_3$** with selected dopants.

Result

- **Rietveld refinement result**





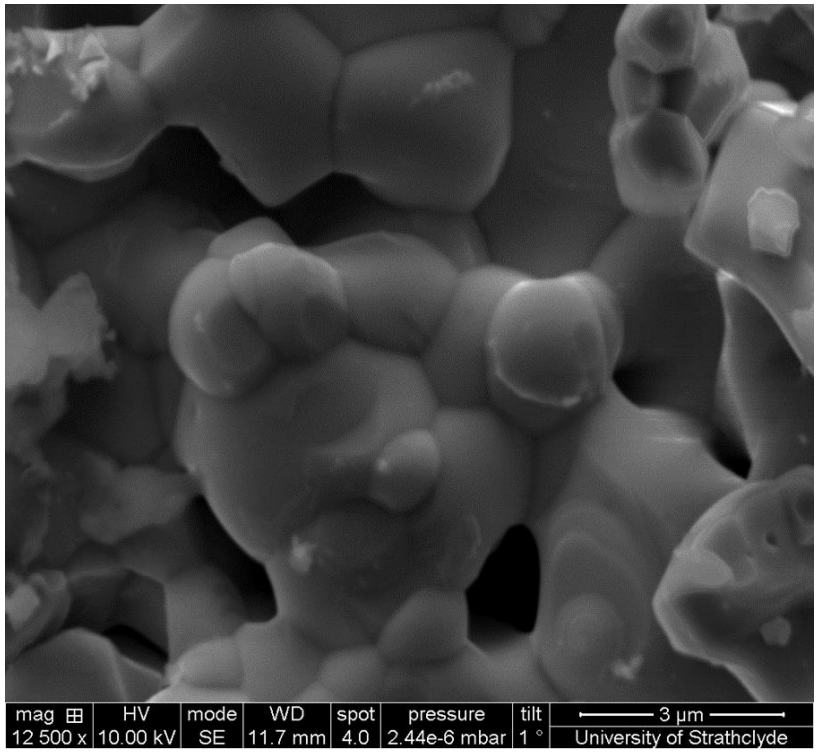
$Sr_{0.95}Ti_{0.3}Fe_{0.6}Cu_{0.1}O_3$ unit cell

Sr0.95Ti0.3Fe0.6Cu0.1O3
Phase fraction: 10.97,
Weight fraction: 97 %,
Microstrain: 606.1
crystallite size: 10.0 μ
a: 3.88228 Å, Volume: 58.514 Å^3

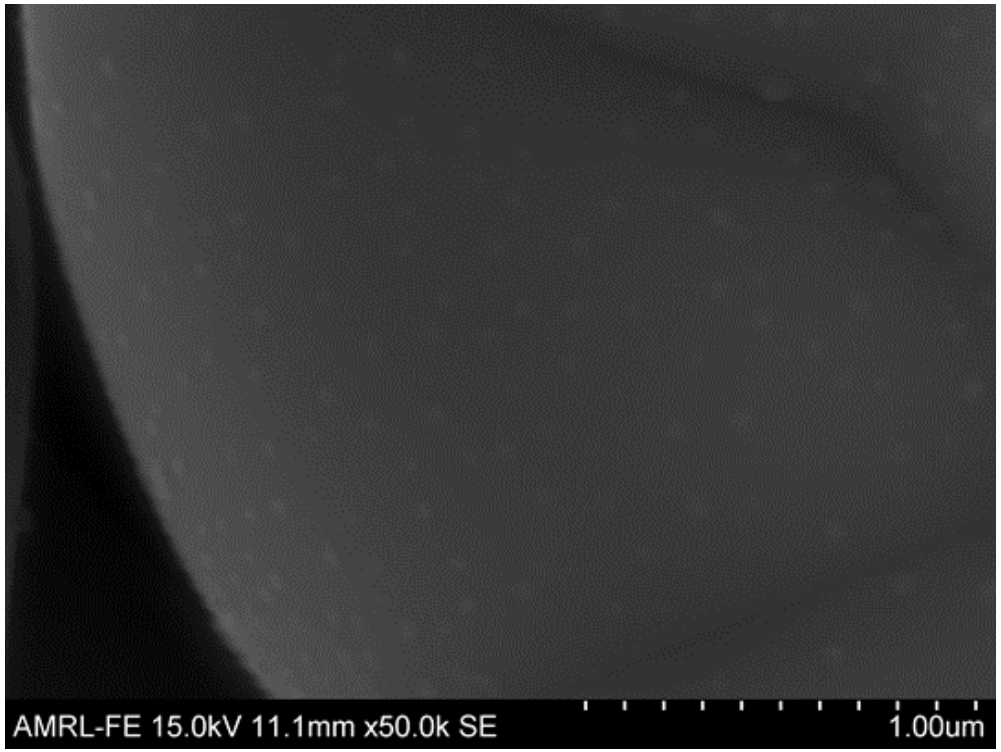
CuO
Phase fraction: 0.18719,
Weight fraction: 2.86 %,
Microstrain: 941.3
Crystallite size: 0.3674 μ

Result

- **Exsolution Observed**



Microstructure of **Sr0.95Ti0.3Fe0.6Cu0.1O3** after sintering



Exsolution in **Sr0.95Ti0.3Fe0.6Cu0.1O3** at **600 ºC** in **1 hr,** after reduction in **5 % H_2**

With exsolution observed at **temperature range of 400 – 600 ºC at 1hr**, **$Sr_{0.95}Ti_{0.3}Fe_{0.6}Cu_{0.1}O_3$** presents a novel perovskite material with fast exsolution process.

Result

- **Step towards further characterization and optimization of the material**

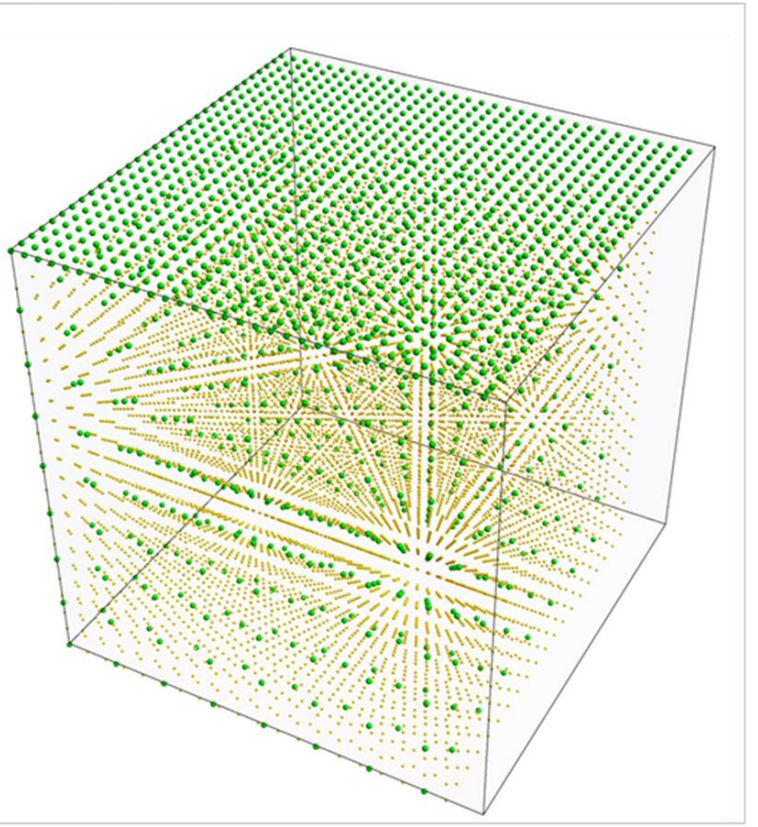
Model Parameters

BsCatsPerUcell :	4
Vocell Size (nm):	100
Cations Radius (nm):	0.3
ExsTime (hrs):	1
ExsTemp (°C):	400
CellParam (nm):	8

Results

Volume of the Vocell:	1 000 000	(nm^3)
Volume of the unit cell:	384	(nm^3)
Number of unit cells within the cube volume:	2604.166667	
Number of cations within the Vocell:	8853.666667	
Number of exsolved particles:	1042.000000	
Number of bulk particles:	521.0000000	

Graphics



Schematics of a **predictive model for the exsolution process** for properties tuning in the synthesized perovskite materials.

Conclusion

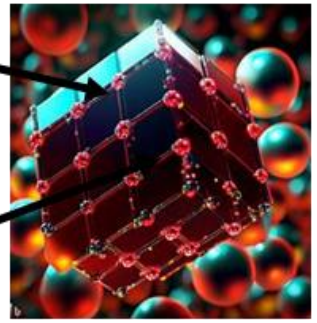
- Achieving exsolution at **400 - 600 °C and 1 hour** in the novel perovskites has shown the possibility of low temperature operation and enhanced durability of RSOCs.
- Electrodes fabricated from the novel perovskites can overcome the electrochemical requirements of RSOCs and enhance mode switching between electrolytic and fuel cell.
- The **predictive model for exsolution process** when completed will facilitate further optimization of the novel perovskites properties for hydrogen production and power generation.

Conclusion

Great Advantage

Anchored nanoparticles

Strained nanoparticles



=

Enhanced activity

Durable nanoparticles

Stable catalysts

Particles properties (shape, size, …) tunability

Fast and **low-temperature exsolution**

400 - 600 °C in 1 hour

=

Great advantage for RSOCs

- ✓ low-temperature operation
- ✓ enhanced mode switching
- ✓ durability
- ✓ electrochemical stability
- ✓ improved efficiency

Further Work

- Exsolution analysis and study of bulk exsolution in the materials;
- Modelling of the exsolution process for performance optimisation;
- Fabrication of RSOCs electrodes; and a RSOCs for testing and benchmarking.

Acknowledgement

I acknowledge

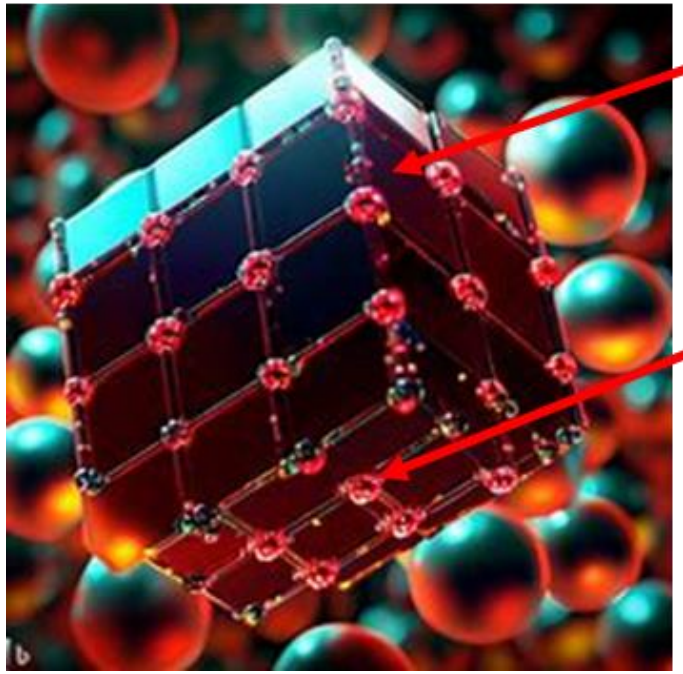
PETROLEUM TECHNOLOGY DEVELOPMENT FUND
PTDF

University of Strathclyde Glasgow

RSE The Royal Society of Edinburgh
KNOWLEDGE MADE USEFUL

Do you think there’re still so much to be answered about exsolution mechanism?

Innovate Material



Perovskite Material

- Properties tuning?
- Exsolution rate?
- …?

Exsolved nanoparticle

- How many?
- Where?
- What size and shape?
- Catalytic activity
- …?

Thank you for listening