DE-FE0031652#

Computationally Guided Design of MULTIPLE Impurities Tolerant Electrode

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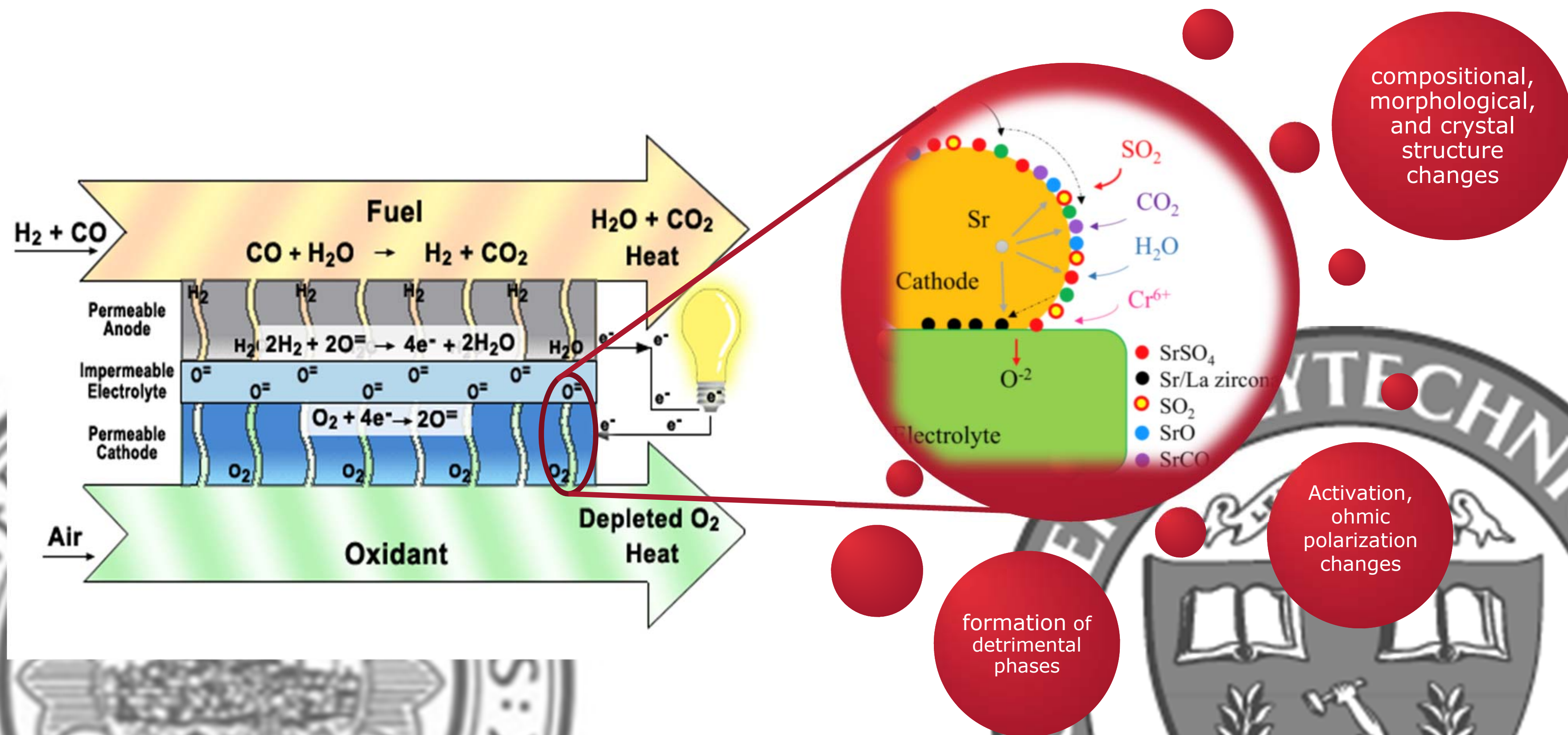
Co-PI: Dr. Srikanth Gopalan (Boston University)

Outline

- Introduction and Project Objectives
- ICME Approach
- PIs Previous Successes on Long-term Degradation
- Project Management
  - Tasks and Deliverables
  - Project Timeline
  - Timetable

Introduction



Slide 3

Office1 original ppt is needed

Microsoft Office User, 9/11/2018

SOFC Development

Decreasing Activation Polarization by Maximizing the Rates of the ORR Reaction

Materials Compositional Design

Reducing Long-term Degradation due to the Effect of Single Air-contained Impurity

External Impurity Getter

GOAL:
Develop The Cathode Material with

1. **High Initial Power Density**
2. **Low Long-term Degradation Rate**

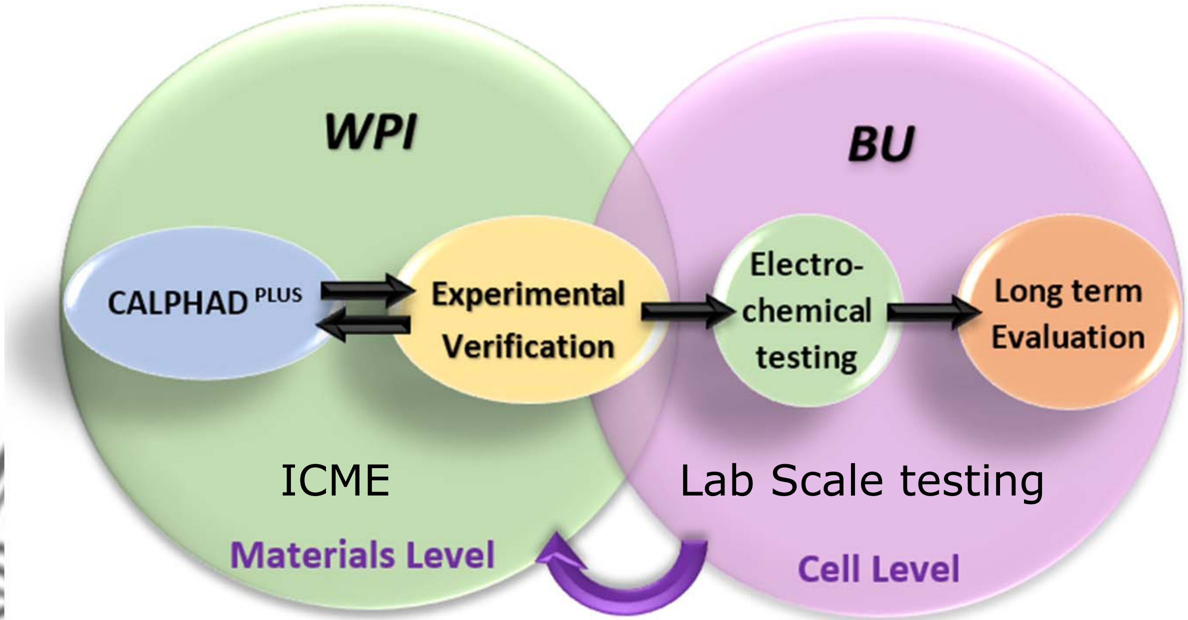
CURRENT LIMITATIONS with Trial and Error Approach:

- Characterization Detection of Nano-sized Secondary Phases
- Difficulty of Doing In-situ or In-operando Observation
- Detailed Reaction Mechanism Verification
- Real Impacts of Multiple Gas Species on Cell/Stack Performance

Novel Integrated Approach and Objectives

Phase I:

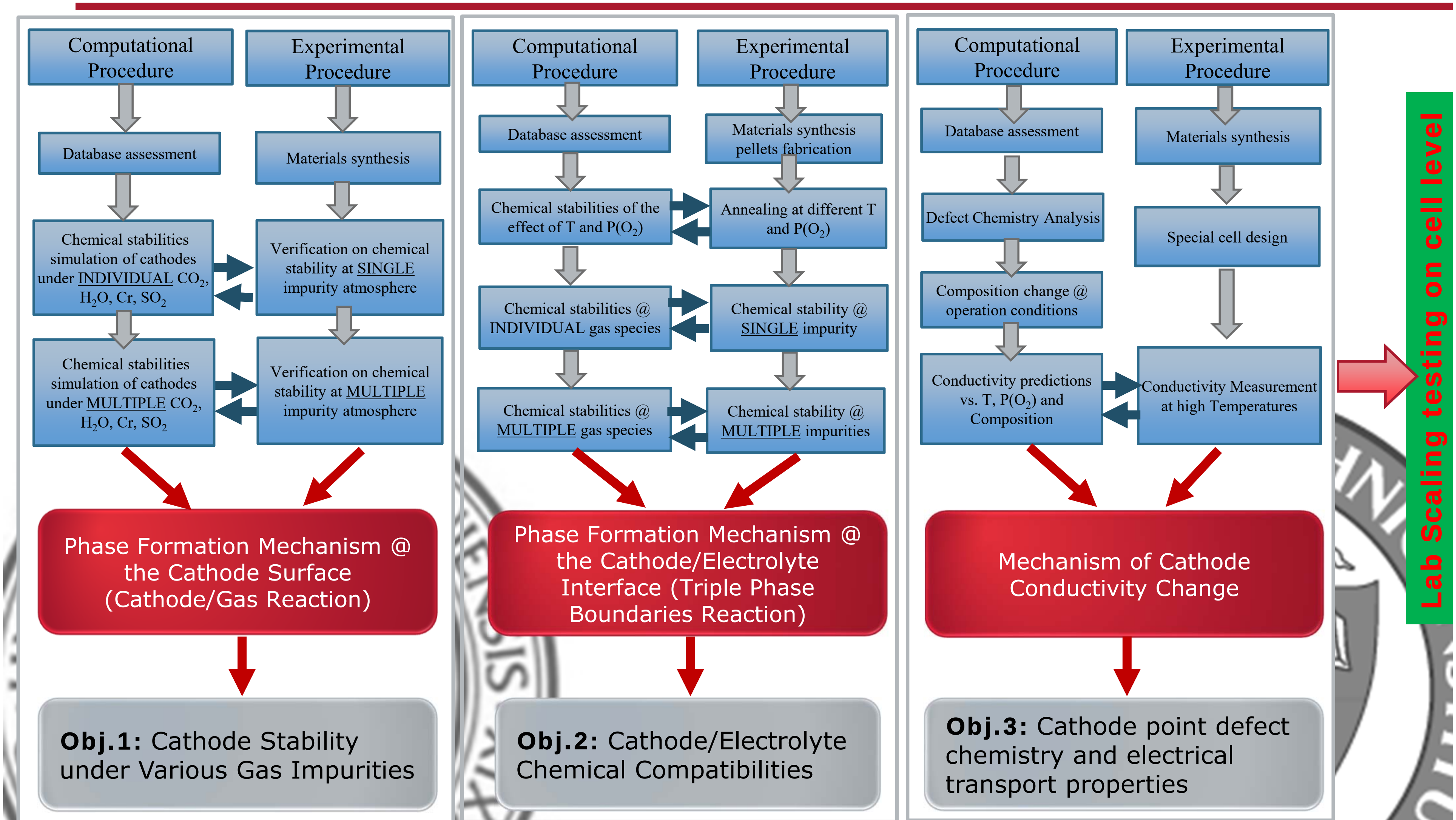
- Achieve the highest power densities of 1.5W/cm^2 at 800ºC
- Achieve a degradation rate of 0.4%/1000hrs under realistic operating conditions with simultaneously present, MULTIPLE impurities at the cell level.



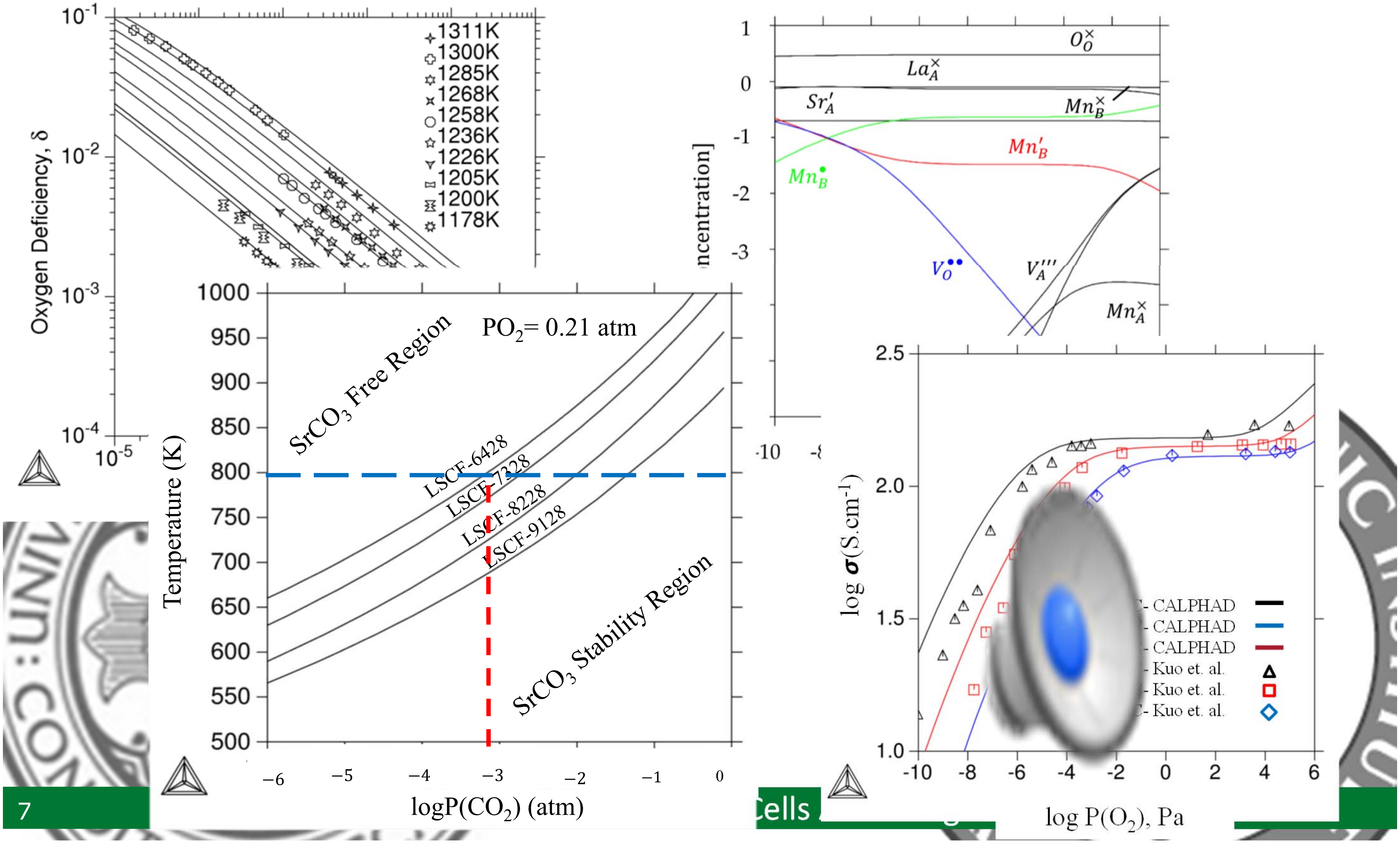
Phase II:

- Achieve a degradation rate of 0.1%/1000hrs at the stack level

ICME Approach at Materials Level

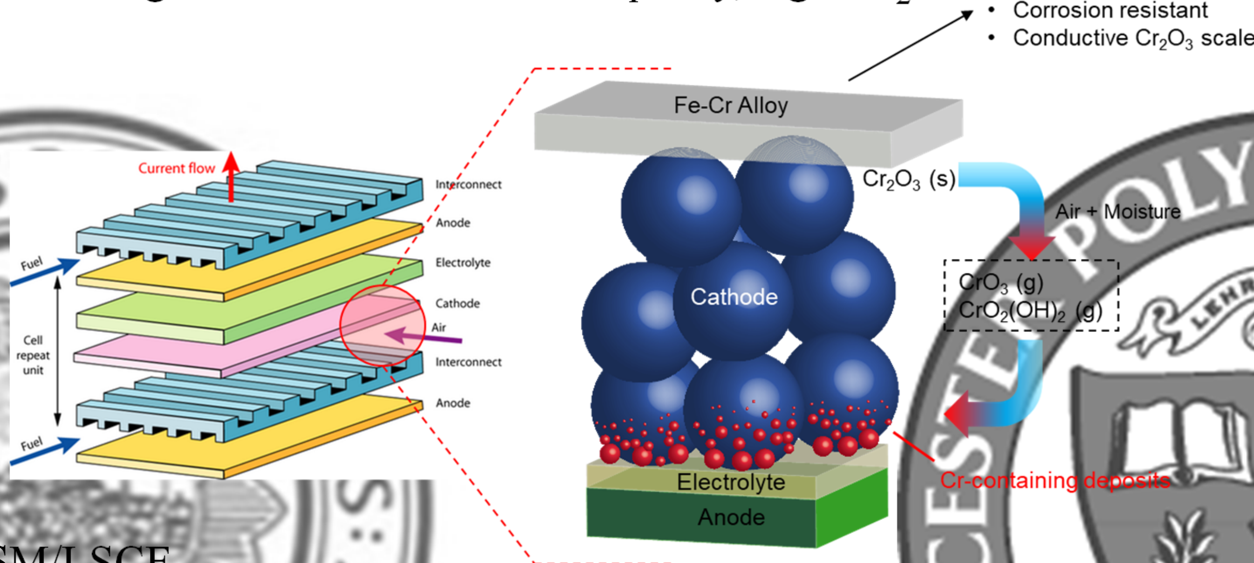


Modeling Prediction Capabilities



Literature review

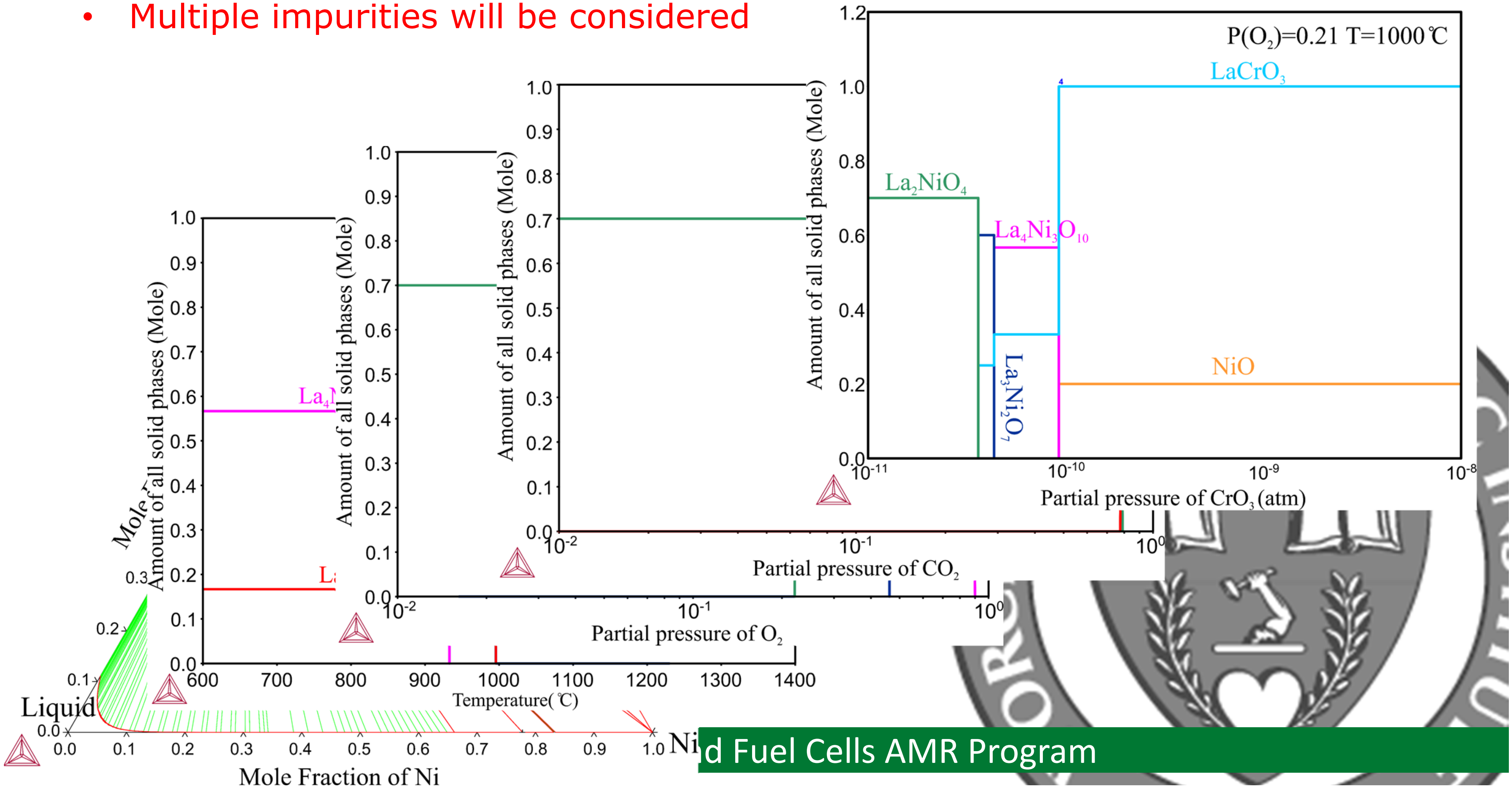
- ❖ Impact of gas impurities on different cathode materials
  - ➢ LNO (promising cathode)
    - ✓ Mixed Ionic and Electronic Conductor
    - ✓ Good performance at intermediate temperature
    - ✓ Higher resistance to some impurity, e.g. CO_2



  - ➢ LSM/LSCF
    - ✓ Traditional cathode (considered as benchmark)

Modeling results So Far

- Thermodynamic database available for LNO
- Individual parameter study (T, O2, CO2, Cr)
- Multiple impurities will be considered

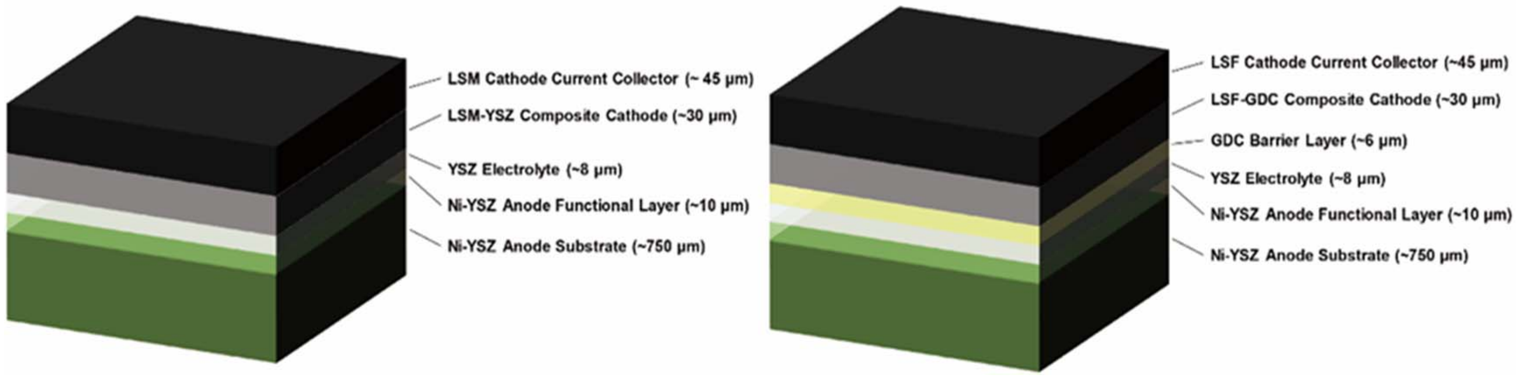


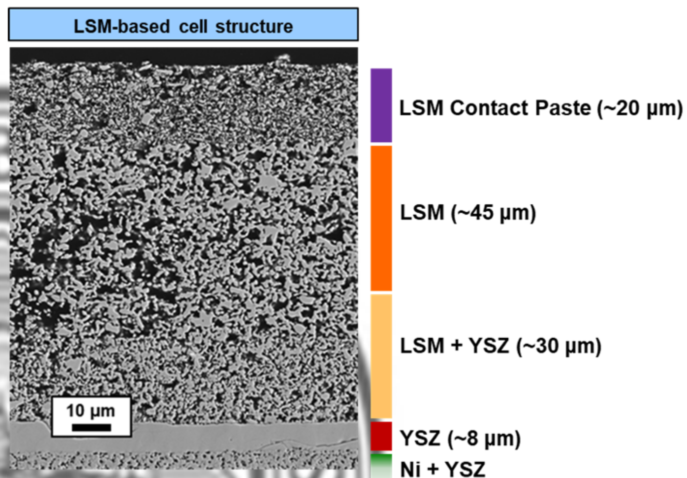
Experimental Plan (Thermodynamic Stability)

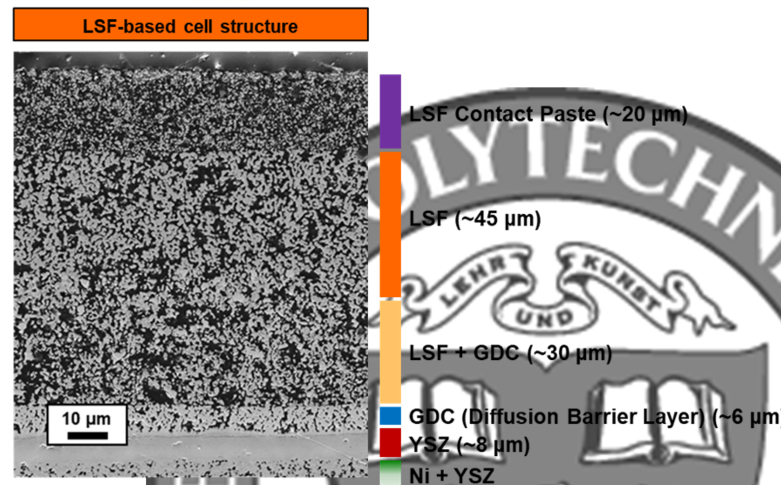
- Impact of different gas impurities
  - Single impurity
    - CO_2
    - H_2O
    - SO_2
    - Cr
    - Si
  - Multiple Impurities

- Experimental plan based on the Literature review
  - LNO/LSM/LSCF + single impurity (CO_2/Cr + dry air)
  - LNO/LSM/LSCF + Multiple impurities (Cr+H_2O, CO_2+H_2O, etc)

Experimental Investigation (Cell)



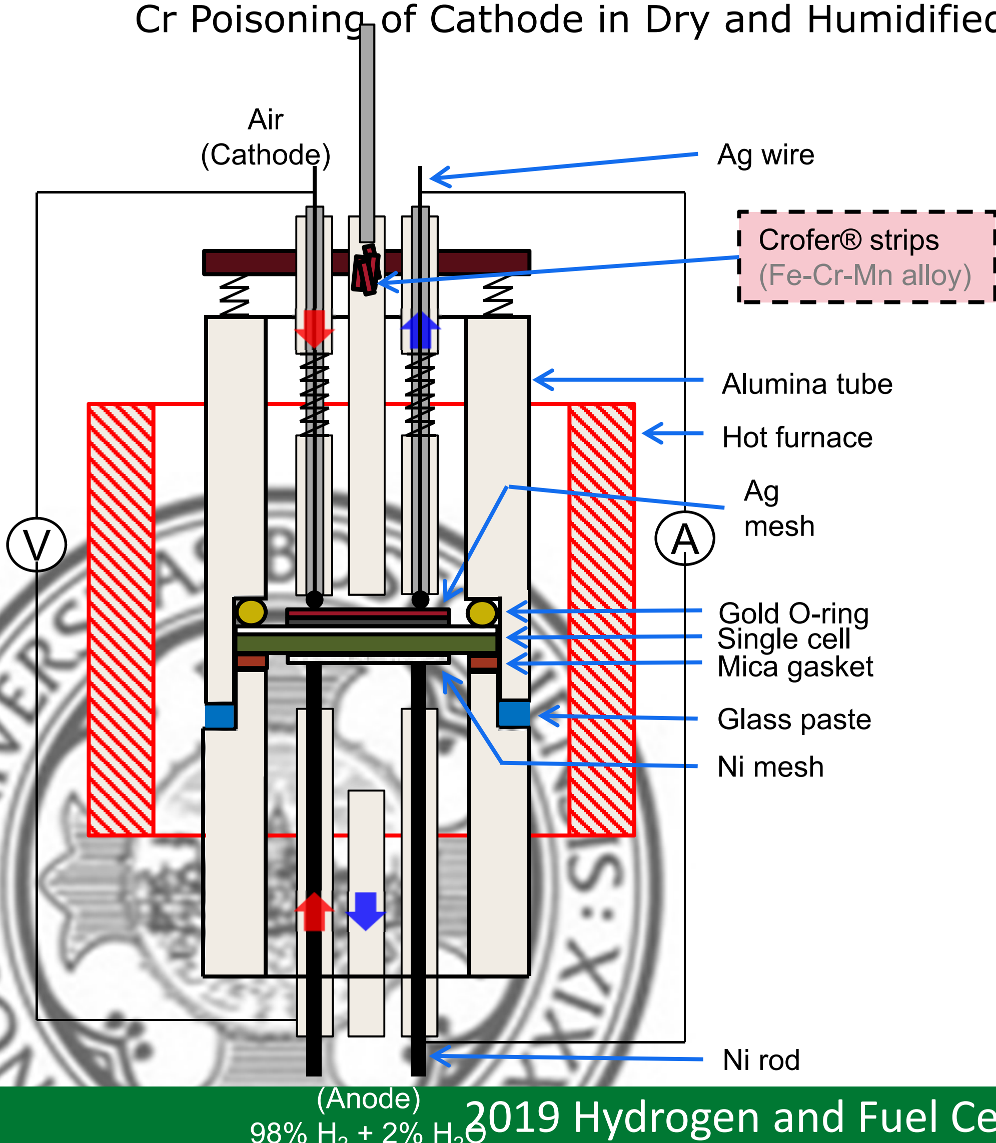


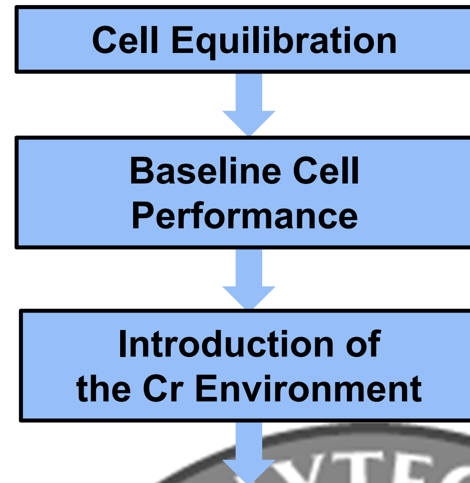


LSM: $(La_{0.8}Sr_{0.2})_{0.95}MnO_{3-x}$
LSF: $(La_{0.8}Sr_{0.2})_{0.95}FeO_{3-x}$
GDC: $(Gd_{0.10}Ce_{0.90})O_{2-x}$

PIs PREVIOUS SUCCESS ON LONG-TERM DEGRADATION

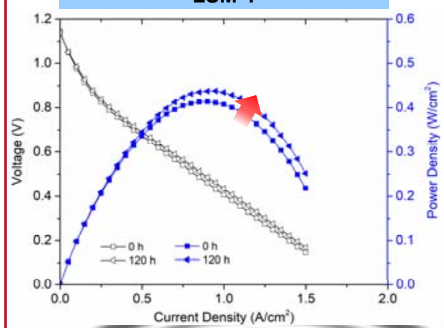
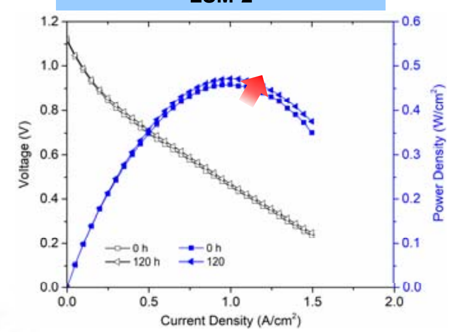
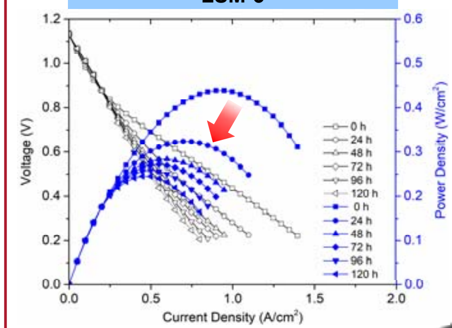
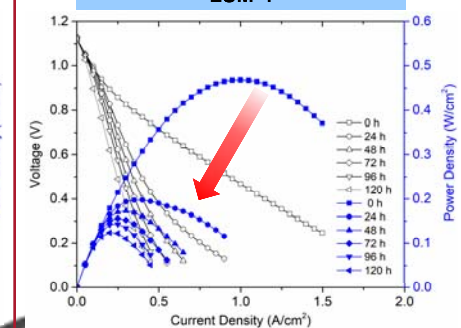
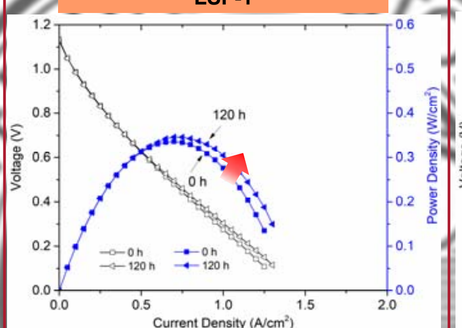
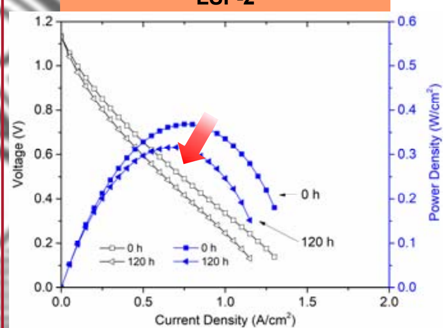
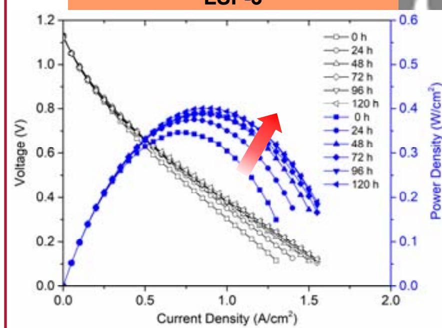
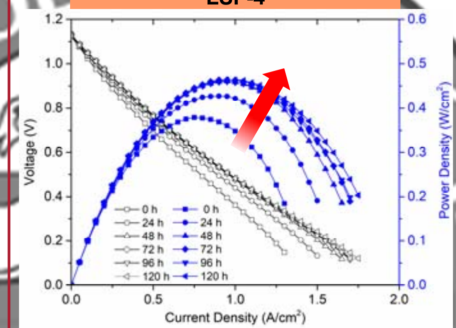
Cr Poisoning of Cathode in Dry and Humidified Air by **Co-PI Srikanth Gopalan**



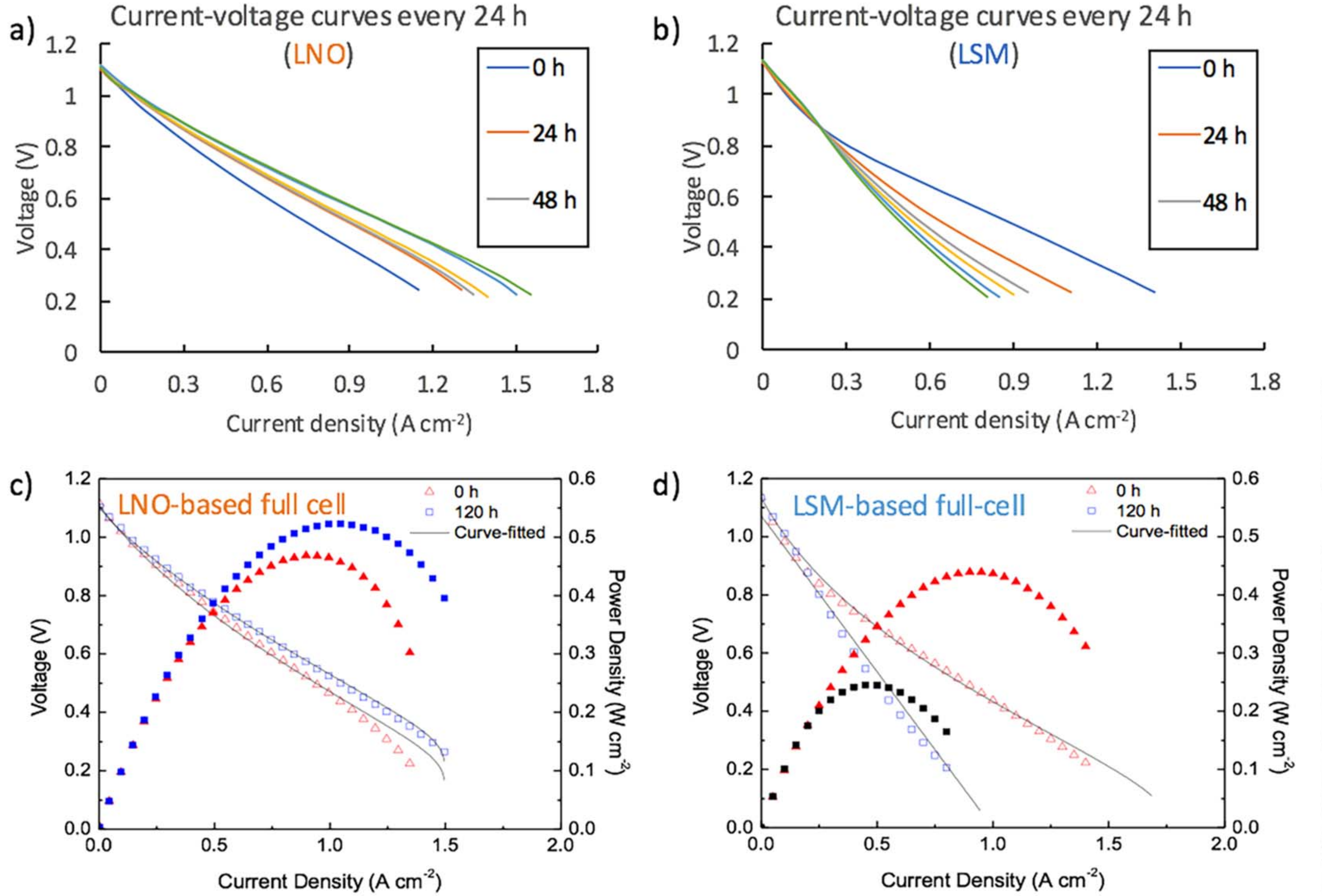


Cell	Cathode Atmosphere	Current Condition
Cell 1	Dry Air	Open Circuit (0 A/cm²)
Cell 2	Dry Air	Galvanostatic (0.75 A/cm²)
Cell 3	Humidified Air (10% H_2O)	Open Circuit (0 A/cm²)
Cell 4	Humidified Air (10% H_2O)	Galvanostatic (0.75 A/cm²)

Electrochemical Degradation (Benchmark)

	Condition 1: Dried Air + OCV	Condition 2: 10% Humidified Air + OCV	Condition 3: Dried Air + 0.5 A/cm²	Condition 4: 10% Humidified Air + 0.5 A/cm²
LSM-Based cells	LSM-1 	LSM-2 	LSM-3 	LSM-4 
LSF-Based cells	LSF-1 	LSF-2 	LSF-3 	LSF-4 

Electrochemical Degradation: LSM vs LNO



Project Timeline

Task/Milestone	Project Timeline							
	Q1	Q2	Q3	Q4	Q5	Q6	Q7	Q8
Task 1. Project Management and Planning								
D1: Quarterly Reports	•	•	•	•	•	•	•	•
D2: Annual Progress Reports				•				
D3: Final Technical Report								•
Task 2. Literature Review of Existing Experimental Data								
M1: Find out the experimental data from literature		■						
Task 3. CALPHAD^{PLUS} simulations								
Subtask 3.1 Simulations of cathode stability under various gas impurities								
Subtask 3.2 Simulations of cathode/electrolyte chemical compatibilities								
Subtask 3.3 Simulations of defect chemistry and electrical transport properties								
M2: recommend a series of cathode materials for experimental investigation								

We are here!

Project Timeline

Task/Milestone	Project Timeline							
	Q1	Q2	Q3	Q4	Q5	Q6	Q7	Q8
Task 4. Experimental verification in WPI								
Subtask 4.1 Materials synthesis								
Subtask 4.2 Chemical stabilities under various gas impurity conditions								
Subtask 4.3 Conductivity relaxation experiments								
M3: Recommend cathode materials for cell testing								
Task 5. Fabrication of Single Cells Using the proposed cathode								
Task 6. Electrochemical Testing and Polarization Modeling								
M4: Select the final cell to do the long-term degradation test								
Task 7. Long-term degradation test								

Acknowledgement

- Financial support from DOE (DE-FE0031652)
- Program manager Venkat K. Venkataraman
- Help from Ruofan Wang, Yiwen Gong, Uday Pal and Soumendra Basu

Timetable

Number	Task	Description
D3	Task 2	Experimental data from available literature (Feb. 2019)
D4	Subtask 3.1	Simulations of cathode stability under various gas impurities (Dec. 2018)
D5	Subtask 3.2	Simulations of cathode/electrolyte chemical compatibilities (Jan. 2019)
D6	Subtask 3.3	Simulation of cathode defect chemistry and electrical transport properties (Mar. 2019)
D7	Subtask 4.1	Materials synthesis (Jul. 2019)
D8	Subtask 4.2	Chemical stabilities under various gas impurity conditions (Oct. 2019)
D9	Subtask 4.3	Electrical conductivity and conductivity relaxation experiment (Dec. 2019)
D10	Task 5	Cell fabrication (Dec. 2019)
D11	Subtask 6.1	Electrochemical testing (Dec. 2019)
D12	Subtask 6.2	Polarization modeling (Feb. 2020)
D13	Task 7.0	Long-term degradation test (Jul. 2020)
D14	Task 1	Final technical report to DOE (Aug. 2020)

ICME Tasks Needed

- Thermodynamic Databases
  - Database Focusing on Perovskite phases *
  - Database Expanded to Consider Gas Impurities *
- Cathode/Electrolyte Compatibility *
- Impact of Gas Impurities
  - Single impurity
    - CO_2 *
    - H_2O *
    - Cr *
    - SO_2 *
  - Multiple Impurities

**: Not systematic but preliminary results available*

OUTCOMES / IMPACTS

- The prediction of the phase stability and electrical properties of cathode;
- A series of cathode candidates will be proposed based on the consideration of various degradation factors simultaneously;
- The cell test at BU on the cell performance and long-term degradation;
- 2 Ph.D. students (one at WPI one at BU) will complete his/her dissertation research;
- A minimum of 3 peer-reviewed publications will be published from this work.

Facilities at WPI & BU

- Thermo-Calc
  - In house La-Ni-Ca-Sr-Co-Cr-Fe-Mn-O-Y-Zr-H-S-C Database
- A suite of electrochemical test equipment including potentiostats and frequency response analyzers
- Electrochemical modeling software – zplot and analytical models
- Cell fabrication hardware

Tasks and Deliverables

Task 1. Project Management and Planning (Zhong, Q1-Q8)

Task 2. Literature Review of Existing Experimental Data (Zhong, Q1-Q2)

Task 3. CALPHAD^{PLUS} simulations (Zhong, Q2-Q3)

- Subtask 3.1 Simulations of cathode stability under various gas impurities
- Subtask 3.2 Simulations of cathode/electrolyte chemical compatibilities
- Subtask 3.3 Simulation of cathode point defect chemistry and electrical transport properties (ionic and electronic conductivities)

Task 4. Materials synthesis and electrical properties (Zhong & Gopalan, Q3-Q6)

- Subtask 4.1. Materials synthesis
- Subtask 4.2. Chemical stabilities under various gas impurity conditions
- Subtask 4.3. Electrical Conductivity and Conductivity Relaxation Experiments

Task 5. Fabrication of Single Cells Using the proposed cathode (Gopalan, Q4-Q5)

Task 6. Electrochemical Testing and Polarization Modeling (Gopalan, Q5-Q6)

- Subtask 6.1 Electrochemical testing
- Subtask 6.2 Polarization Modeling

Task 7. Long-term degradation test (Gopalan, Q5-Q8)