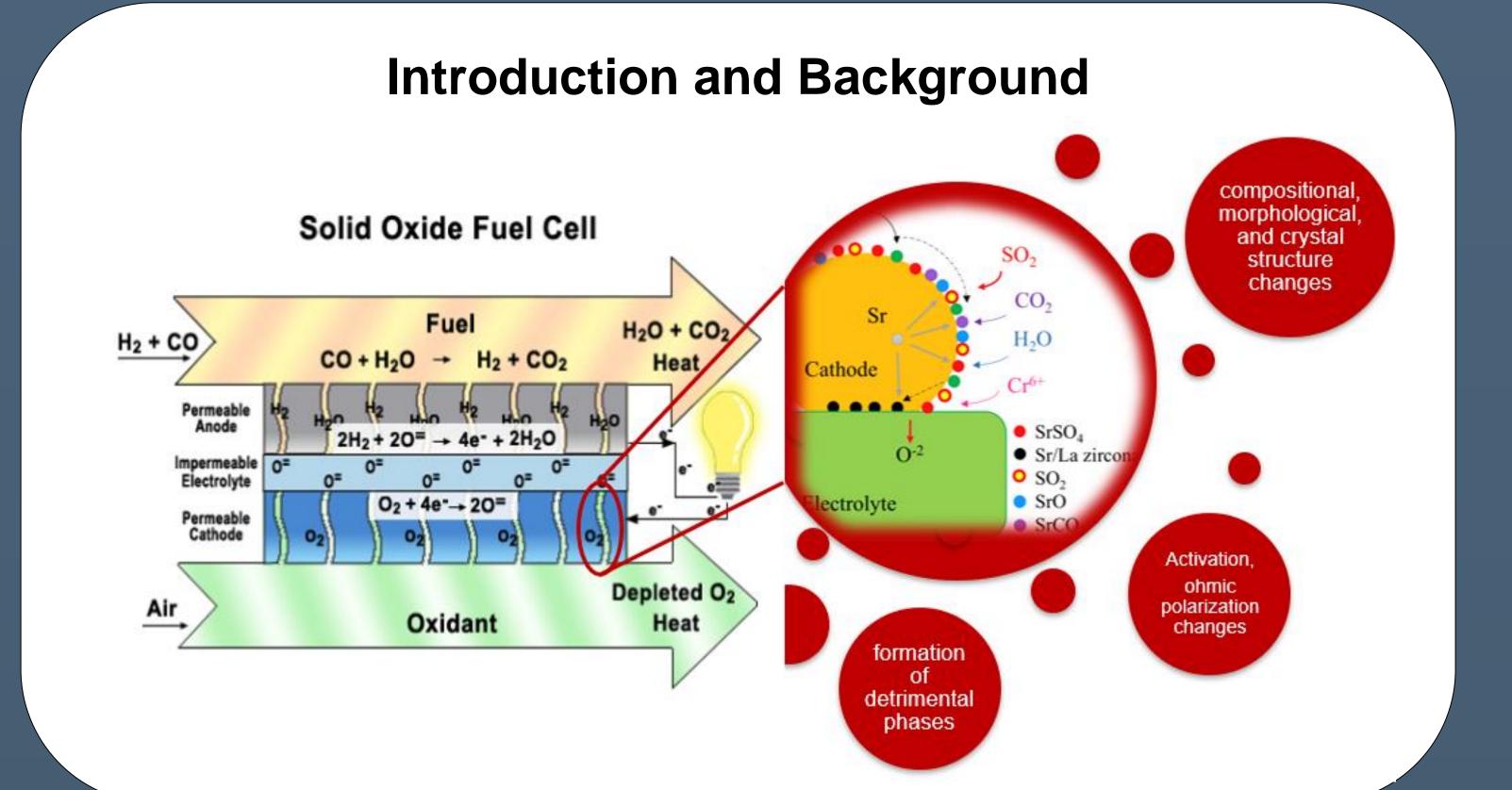


Computationally Guided Design of Multiple Impurities Tolerant Electrode

<u>Rui Wang^a</u>, Lucas R. Parent^b, Srikanth Gopalan^c, Yu Zhong^a

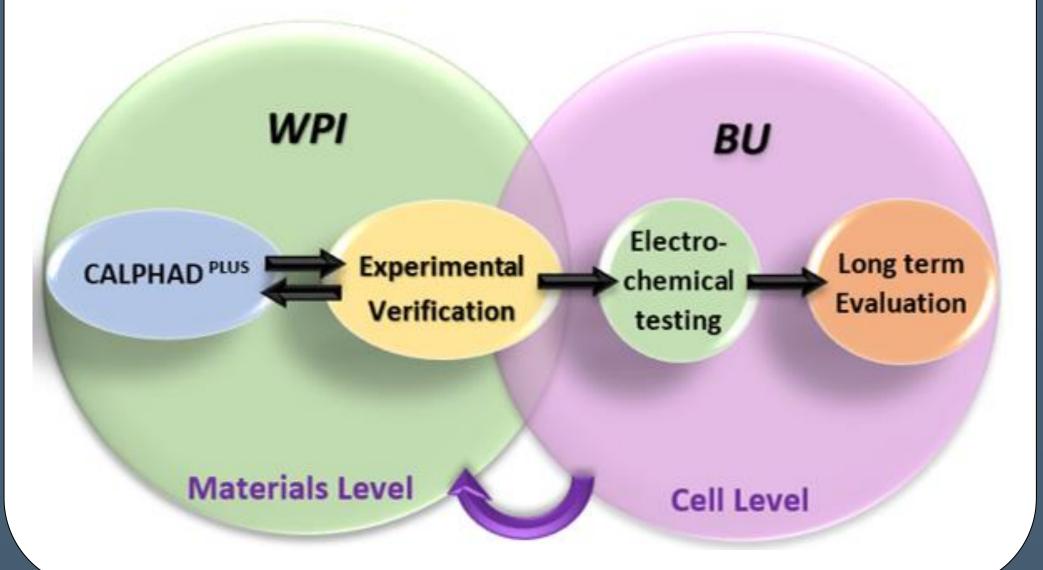
^a Mechanical and Materials Engineering Department, Worcester Polytechnic Institute. ^b Innovation Partnership Building, University of Connecticut. ^C Division of Materials Science & Engineering, Boston University.

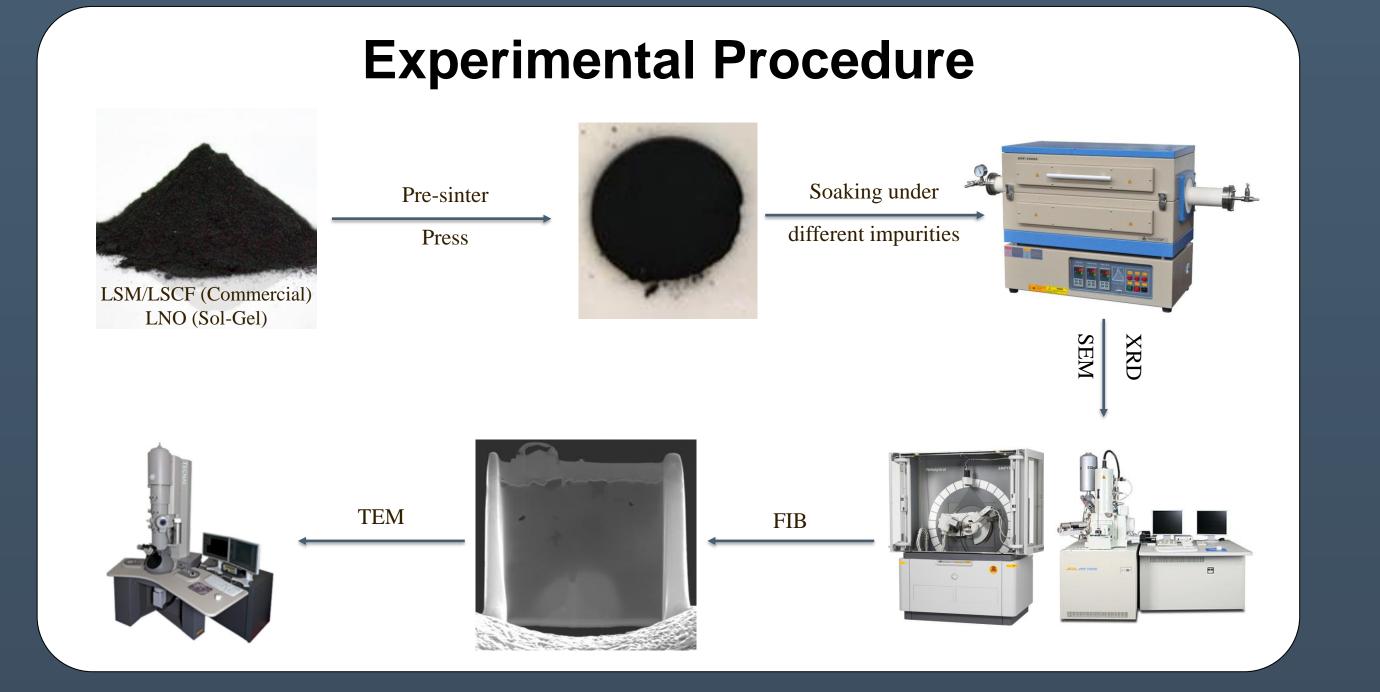




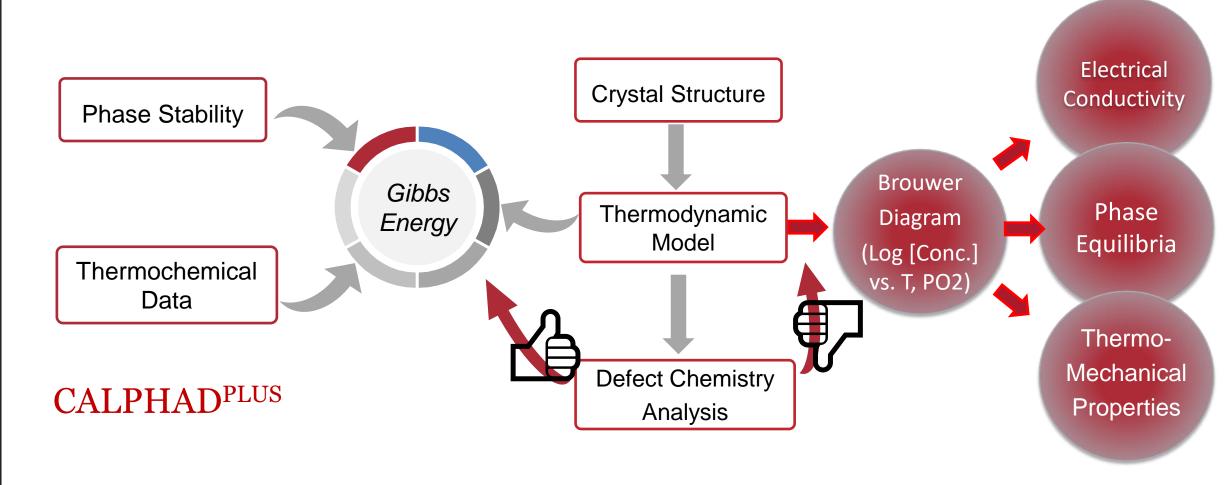
Approach and Objectives

- Investigate the degradation mechanisms of different impurities to the cathode materials.
- Propose tolerant electrodes under different conditions.



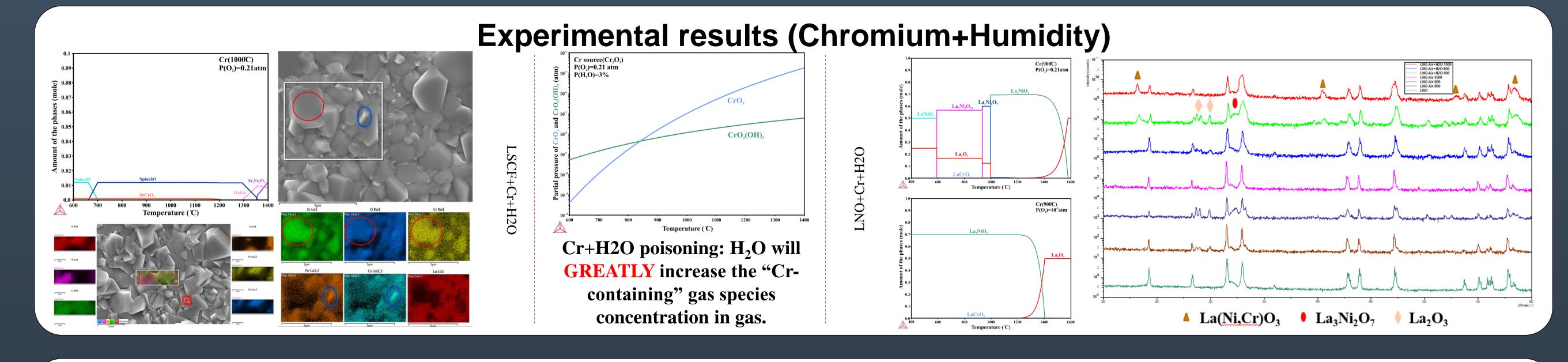


Computational Procedure

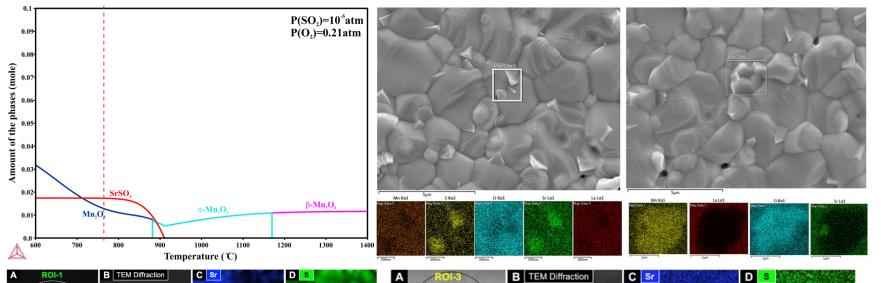


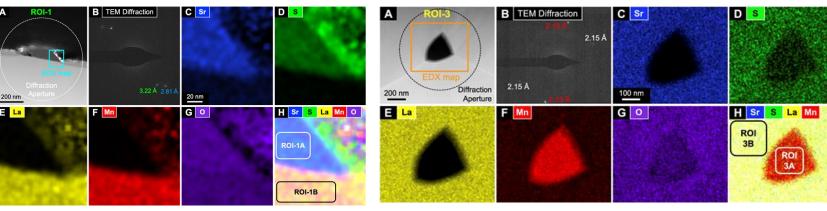
• Database including the perovskite phase/Ruddlesden-Popper phase (LSM, LSCF, LNO)

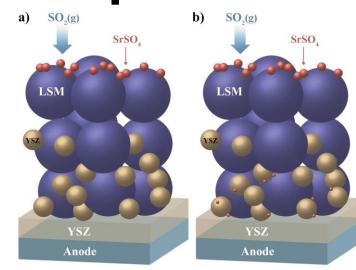
• Database expanded to consider gas impurities (SSUB5)



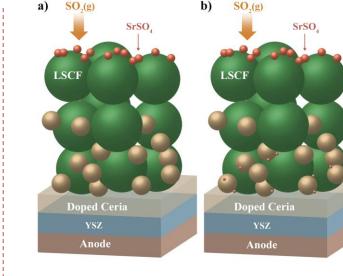
Experimental results (Sulfur)



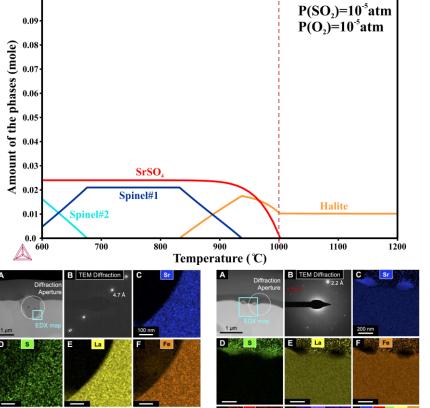


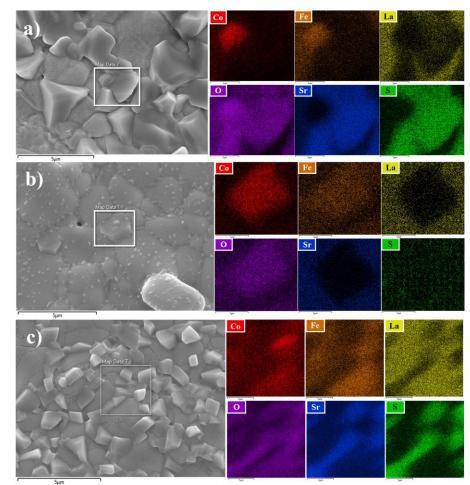


LSM pellets heattreated in 10ppm SO2 balanced with dry air at 800°C for 2 days.

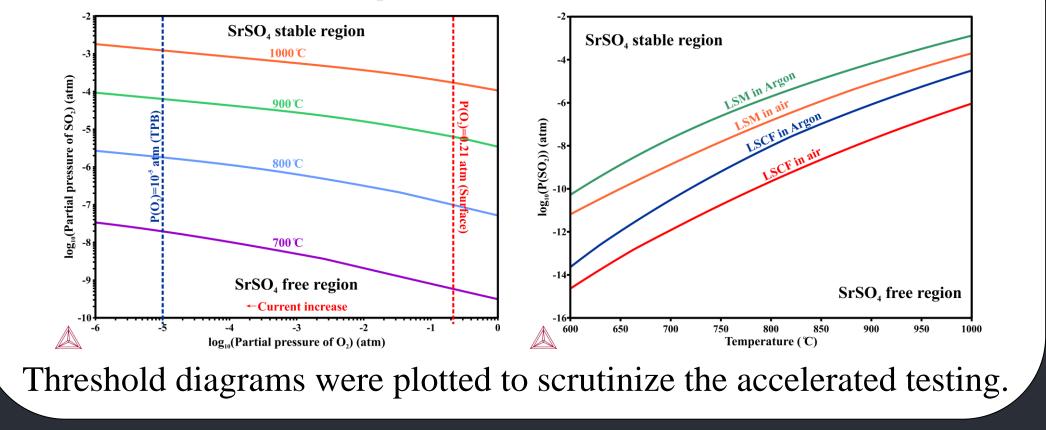


LSCF pellets heat-treated in 10ppm SO2 balanced with dry argon at 1000°C for 2 days.





Computational Results



Summary

Thermodynamic simulations were carried out to understand the effect of multiple impurities to the SOFC cathode materials (LSM, LSCF & LNO)

Acknowledgement

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