

Application of Computational Thermodynamics in Solid Oxide Fuel Cell

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Introduction

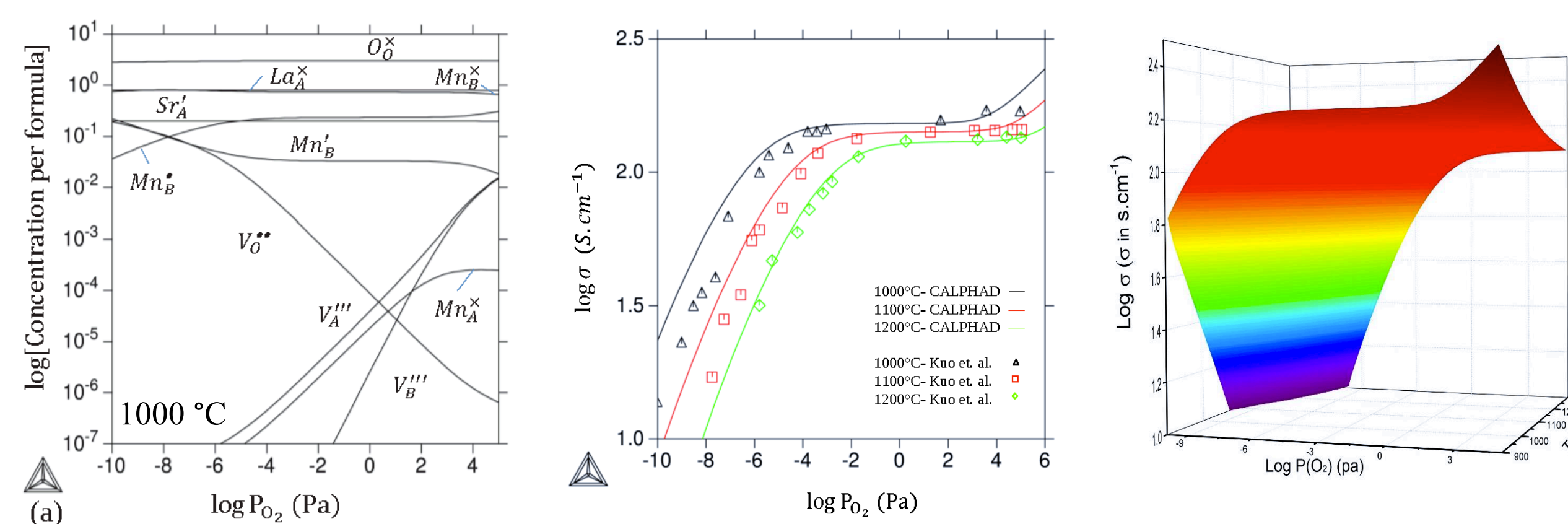
Degradation of the cell components affect the performance of the device due to the:

1. chemical instability of the cathode surface (Region I)
2. the cathode/electrolyte (solid-solid) interfaces at the TPBs (Region II)

Degradation observed in high CO_2 , H_2O , SO_2 , Cr^{6+} partial pressure condition due to the formation of secondary phases such as SrO/SrCO_3 , MnO_x oxides, $\text{Mn}(\text{Mn}, \text{Cr})_2\text{O}_4$, $\text{La}_2\text{Zr}_2\text{O}_7$ (LZO) and SrZrO_3 (SZO). Despite the importance of this fact, degradation mechanism is still not clear.

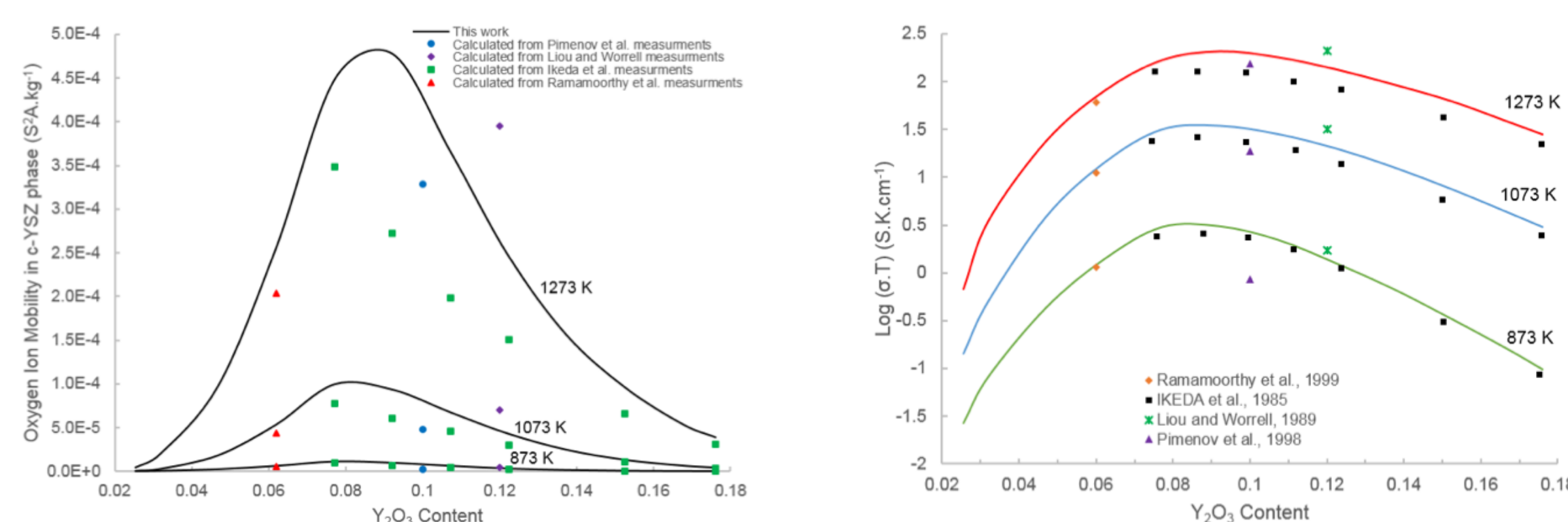


Quantitative Brouwer Diagram and Electronic Conductivity of LSM-20



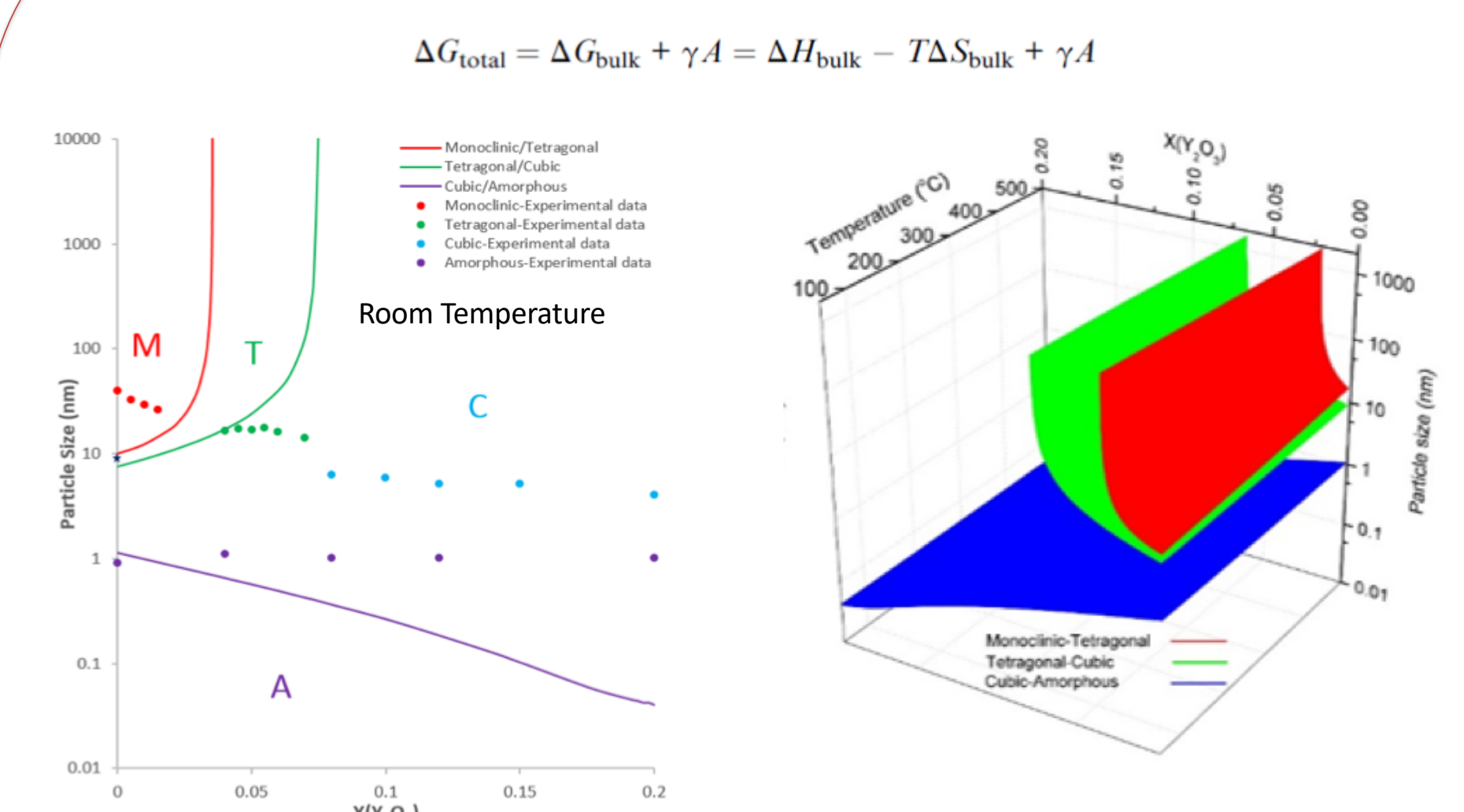
The low ionic conductivity of LSM-20 can be explained with the low vacancy's concentration in the oxygen site.

Ionic Conductivity and Oxygen Ion Mobility in YSZ

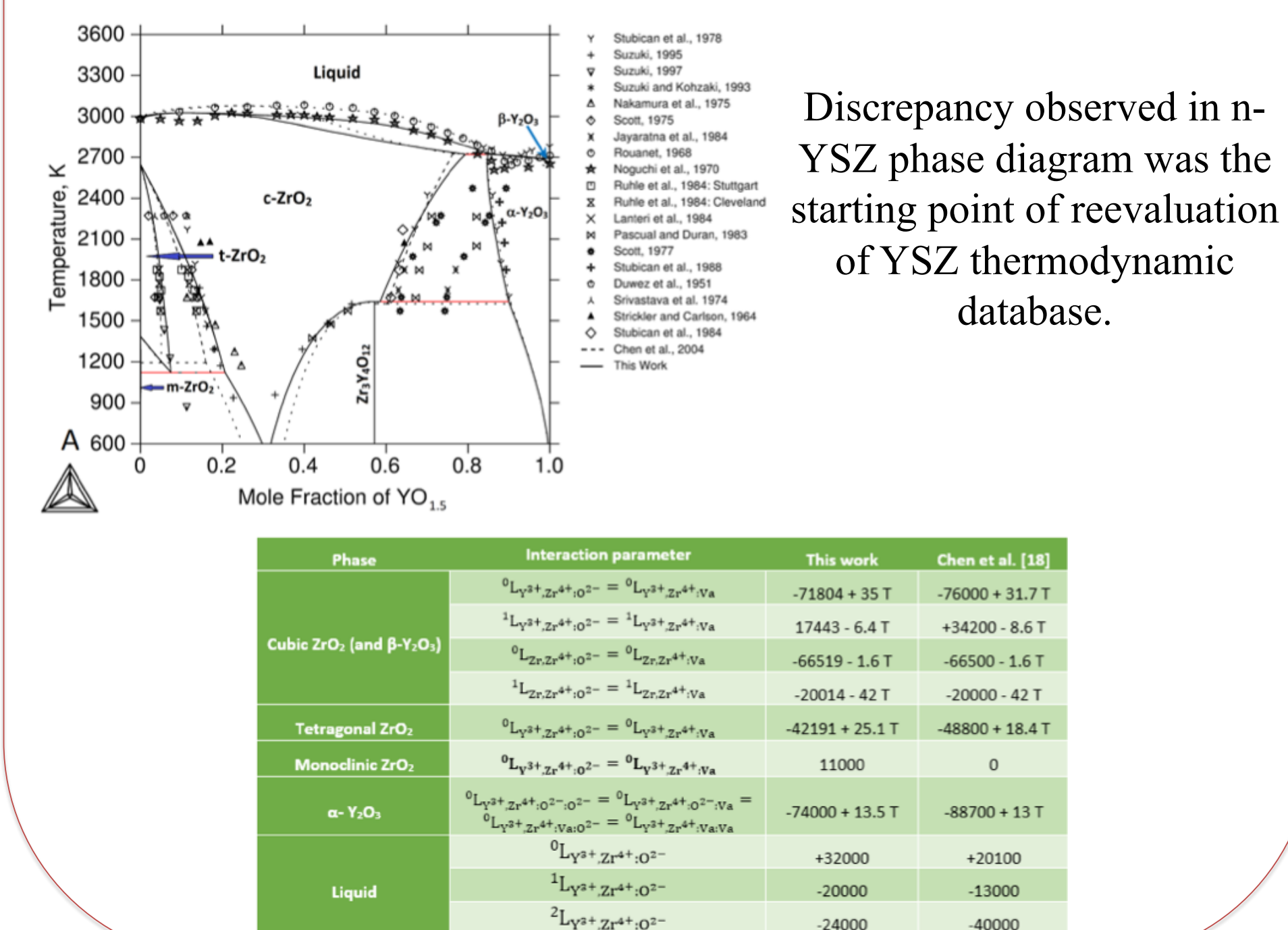


The ionic conductivity, σ , is a function of the charge of carrier, z , the concentration of carrier, n , and the mobility of ions, μ . $\sigma = zn\mu$

n-YSZ Phase Diagram

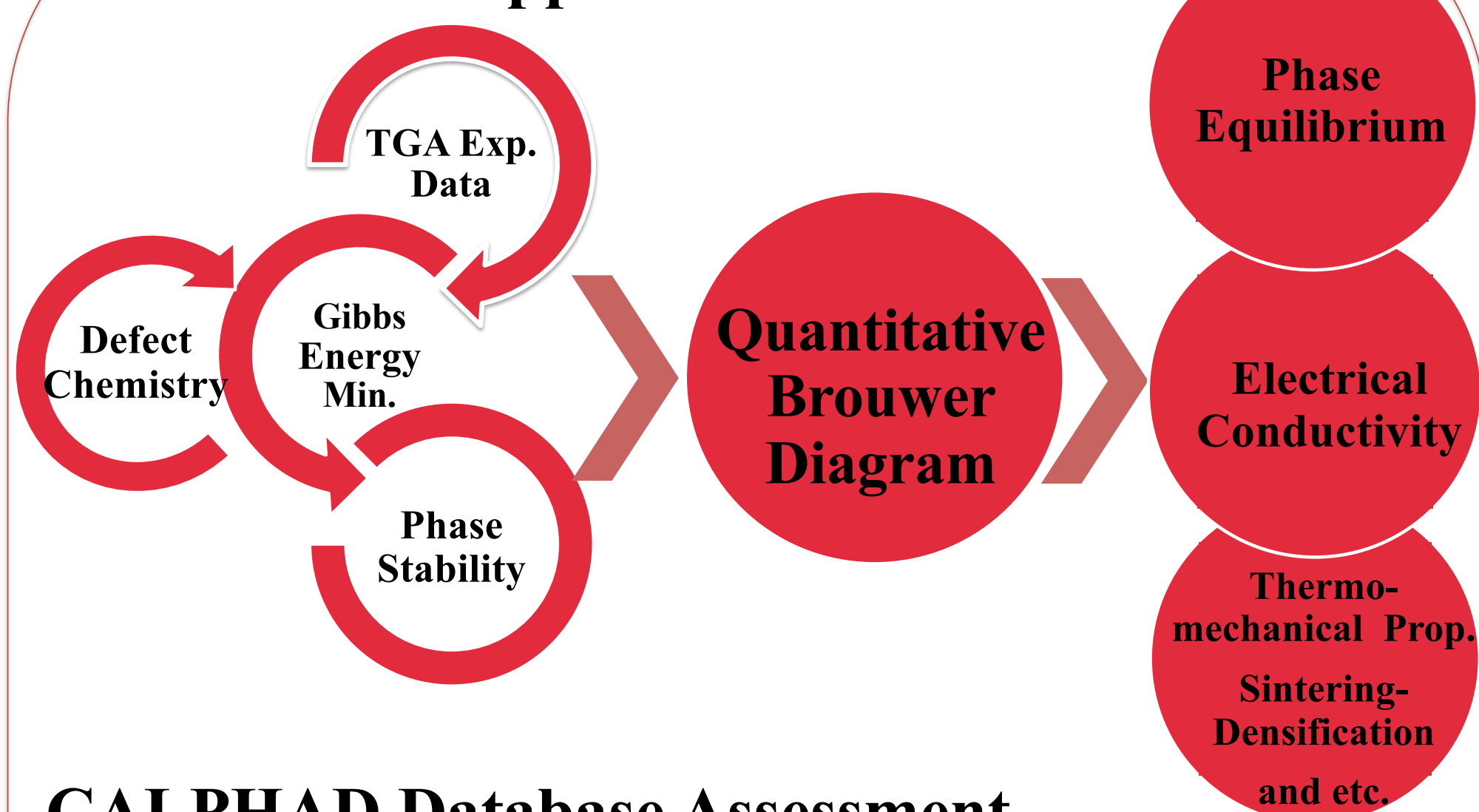


Reassessment of YSZ Thermodynamic Database

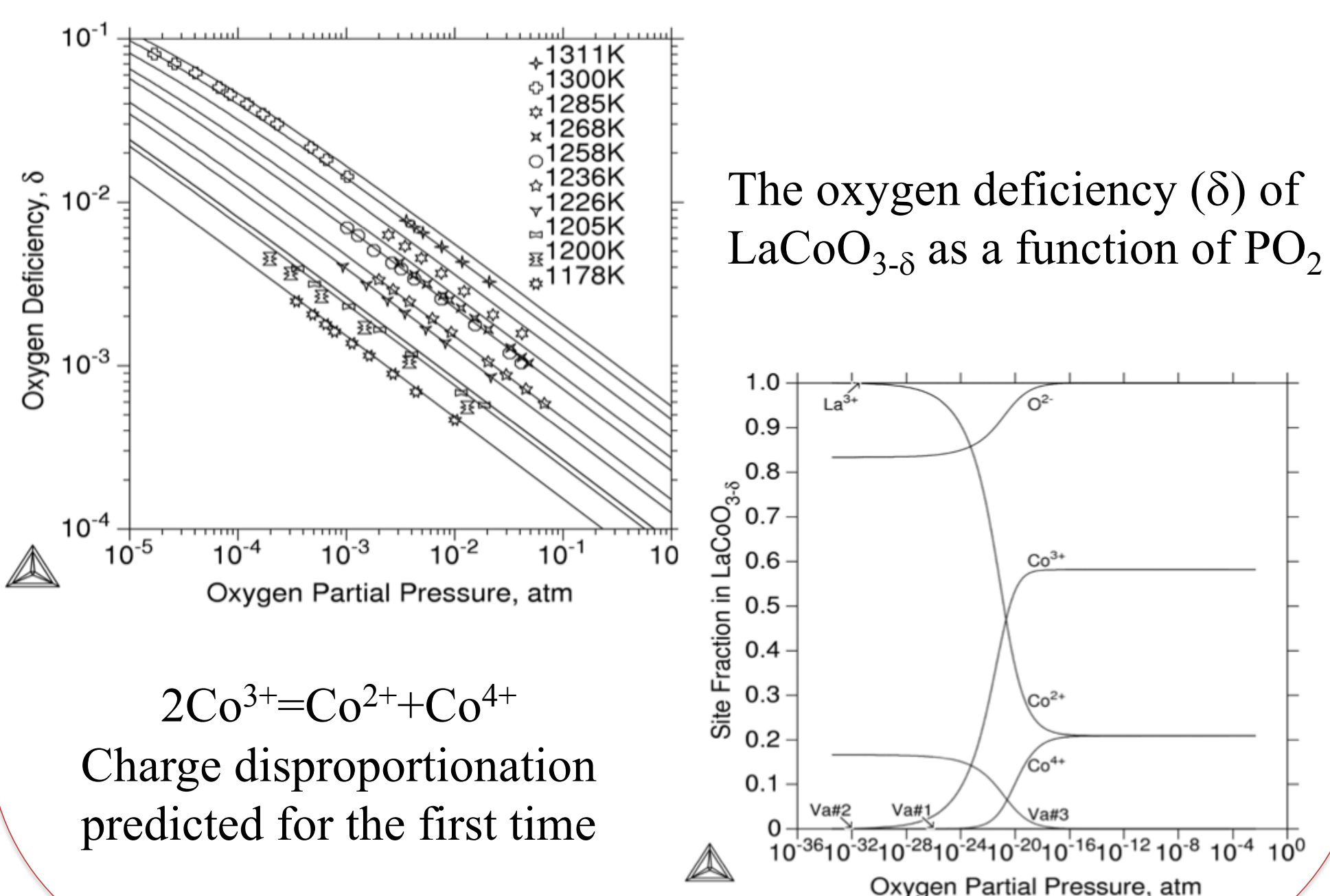


Discrepancy observed in n-YSZ phase diagram was the starting point of reevaluation of YSZ thermodynamic database.

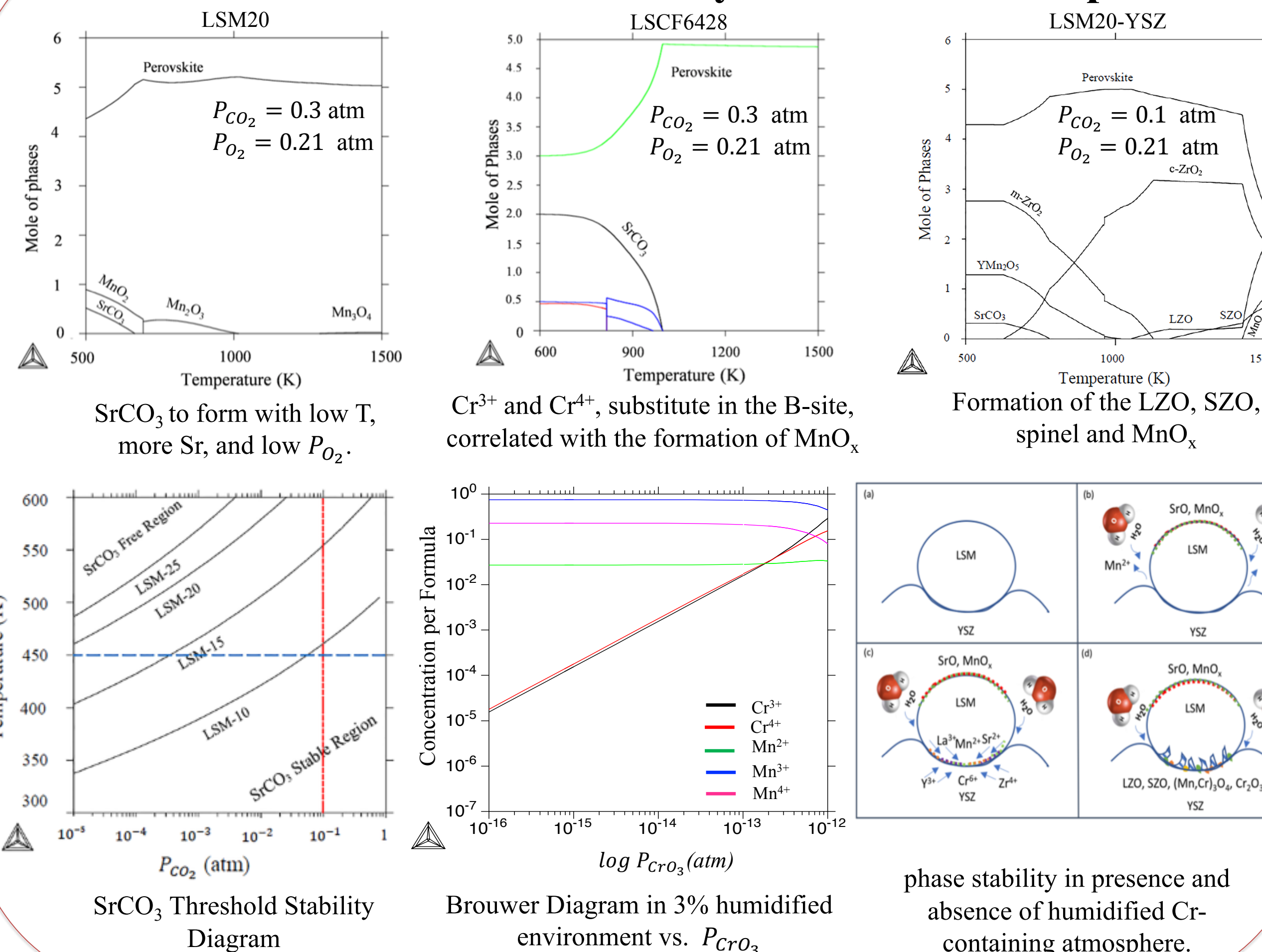
CALPHAD Approach



CALPHAD Database Assessment



LSM20/LSCF6428/8YSZ Stability in Presence of Impurities



Summary

- Computational Thermodynamics can be widely used in Solid Oxide Fuel cell:
- Perovskite and YSZ thermodynamic database development
- Electronic and Ionic Conductivity prediction
- The phase stability prediction of cathode side with the existence of gas impurities
- Phase stability prediction for nano-size particles
- The in-house multicomponent La-Ca-Sr-Mn-Co-Cr-Fe-O-Y-Zr-C-H-S Thermodynamic database can be used for various applications.

Acknowledgement

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