

Steady State Kinetic Isotope Exchange

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About me

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Introduction

The oxygen reduction reaction is an important part of many potential alternative fuels. As the world seeks to reduce the use of fossil fuels more studies are being conducted on these alternative fuel sources, such as fuel cells and lithium-air batteries. We studied the effects of various catalysts on the activation energy of the surface oxygen exchange, which is the rate limiting step of the oxygen reduction reaction.

Relation Sustainable Mg.

Environmental

- By catalyzing this step of the reaction, these sources of alternative energy become more viable, in turn reducing the amount of fossil fuels used.

Economic

- The use of transition metals instead of noble metals reduces the cost of the catalysts.
- The production of efficient alternative energies has the potential of making a profit.

Social

- It also helps meet societies demand for cleaner energies.

State of Knowledge

- Surface oxygen exchange is the rate limiting step of the oxygen reduction reaction.
- Ruddlesden-Popper phase structures favor oxygen exchange.
- B site terminated catalysts of the RP structure are more reactive than A site terminated catalysts.
- Rod structured catalysts are B site terminated along the length of the rod.

Approach

- A theoretical model of activation energies required for each catalyst was produced.
- These catalysts were synthesized using the reverse microemulsion synthesis approach.
- The reactivity of each catalyst was tested using steady state kinetic isotope exchange.

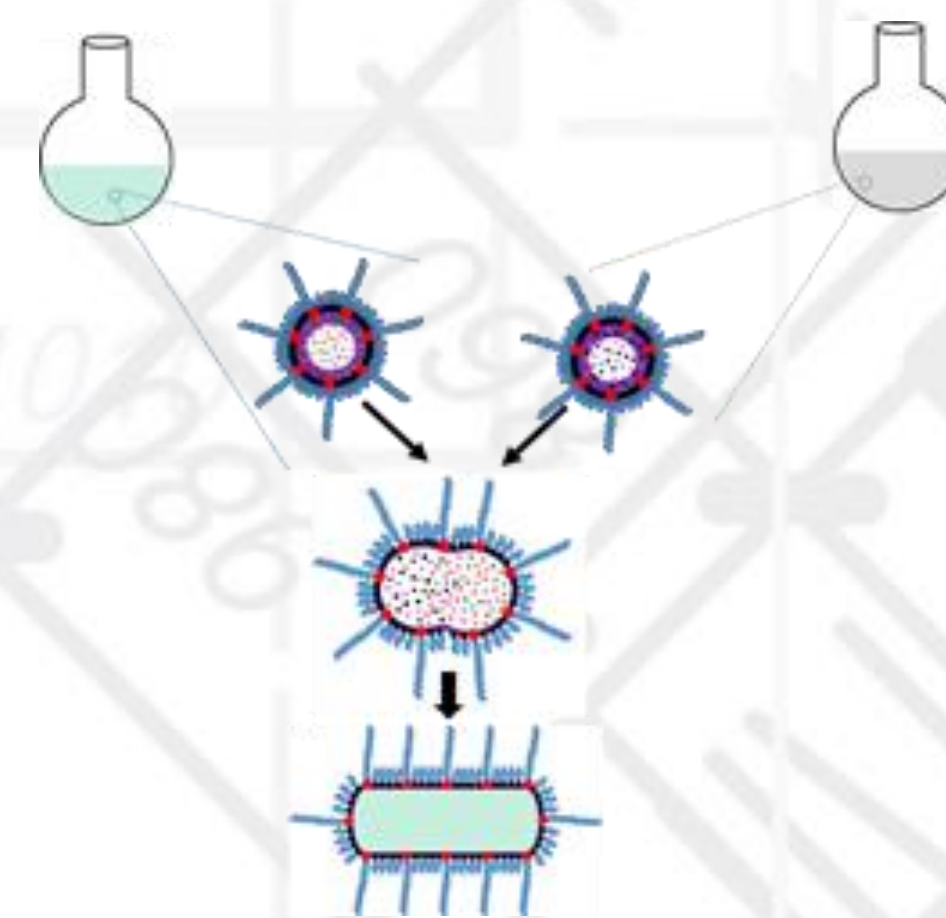


Figure 1: Reverse microemulsion synthesis process

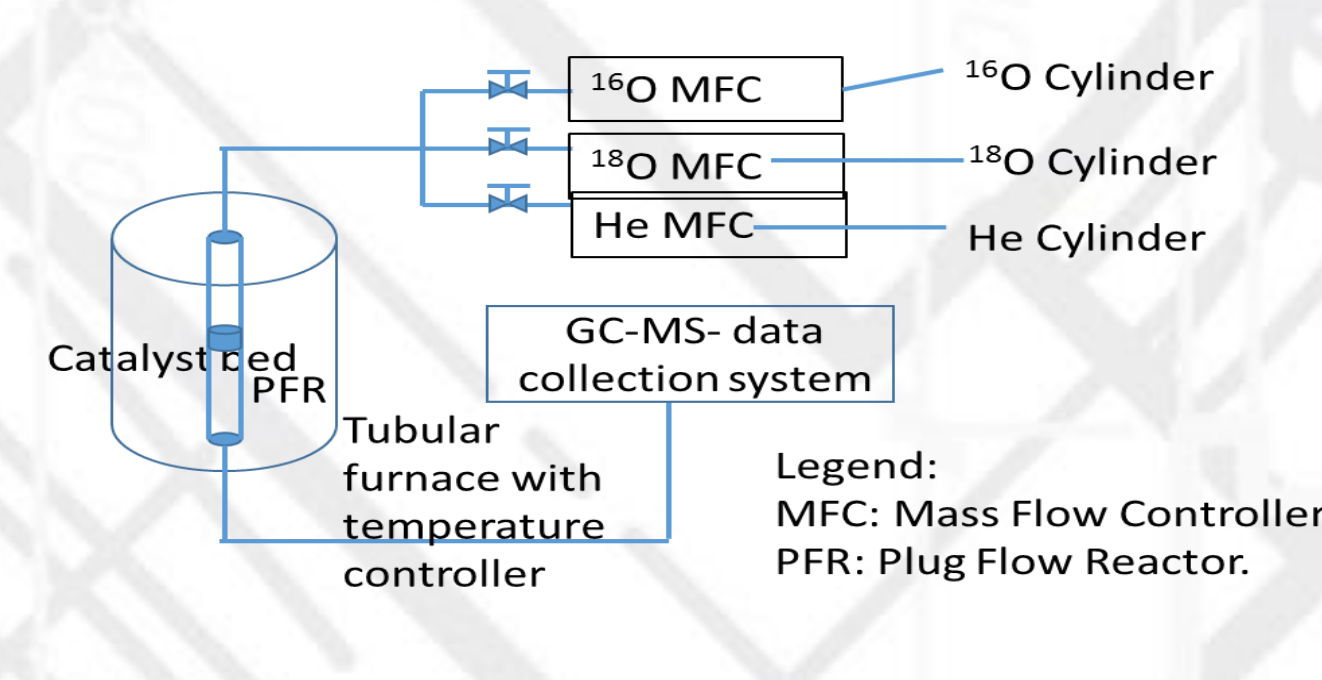


Figure 2: Steady state kinetic isotope exchange diagram

Results

- The activation energies of a number of catalysts were determined.
- $\text{La}_2\text{Ni}_0.5\text{Co}_0.5\text{O}_4$ was the most reactive catalyst as predicted.

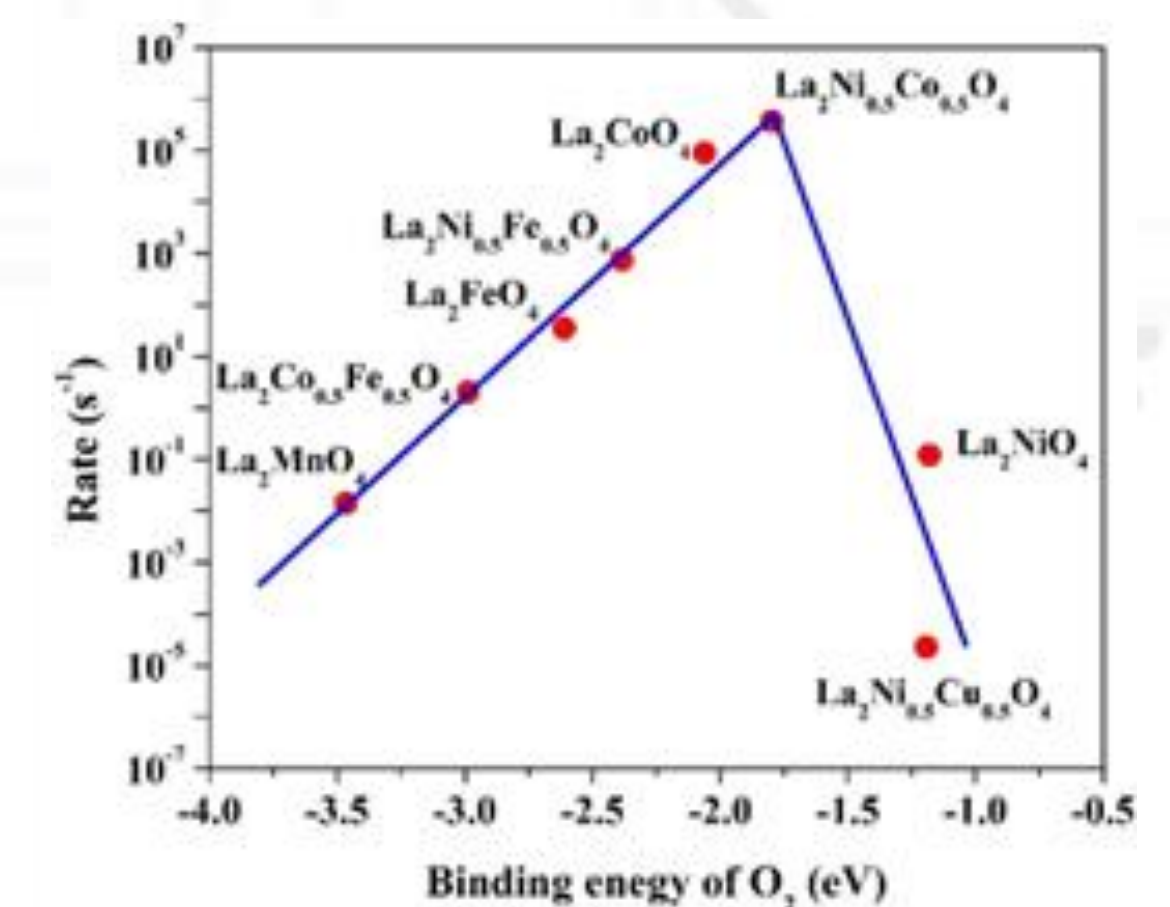


Figure 3: Graph of theoretically determined rates of reaction of various catalysts that were later tested.

Conclusions

- LNO doped in Cobalt results in the most reactive catalyst for surface oxygen exchange and the other catalysts tested more or less followed the predicted trends. This accuracy shows that the reactivity and activation energies of Ruddlesden-Popper catalysts can be predicted and that these predictions can be used to find more reactive and efficient catalysts in the future.

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References

1. Ma, X.; Carneiro, J. *ACS Catal.* **2015**, *5*, 4013-4019
2. Ma, X.; Wang, B. *Chem. Commun.* **2015**, *51*, 137-140
3. Lee, Y.; Lee, D. J. *Phys. Chem. Lett.* **2017**, *7*, 244-249

