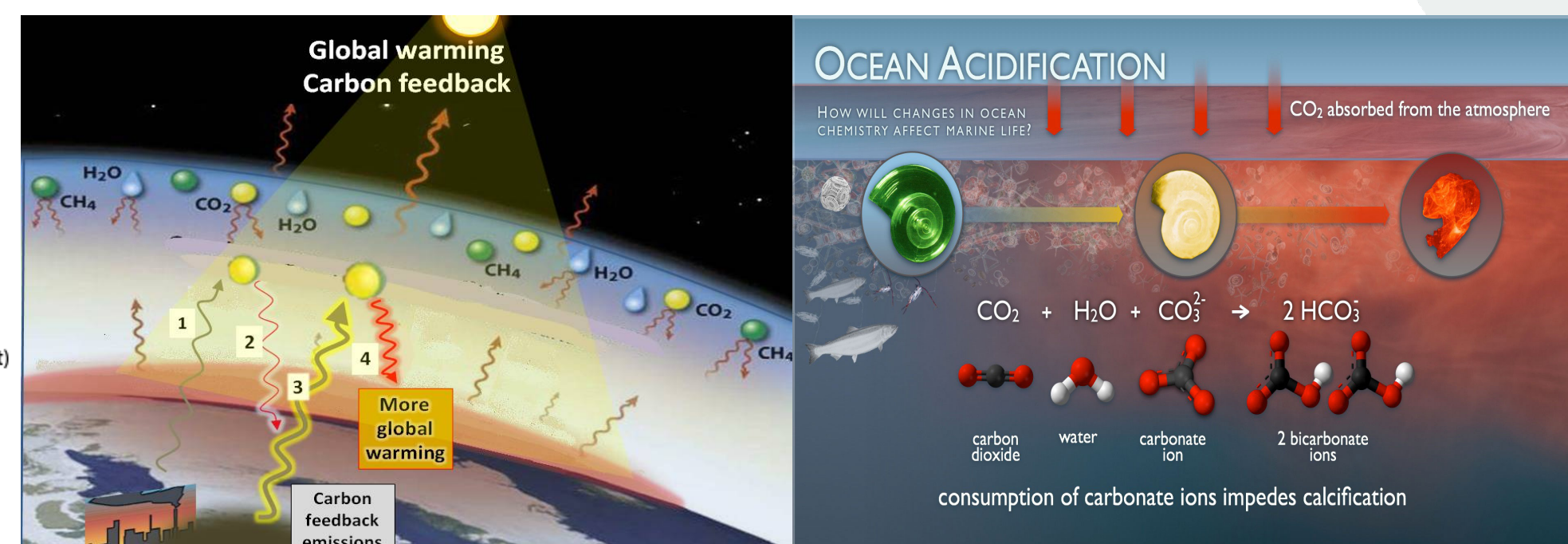
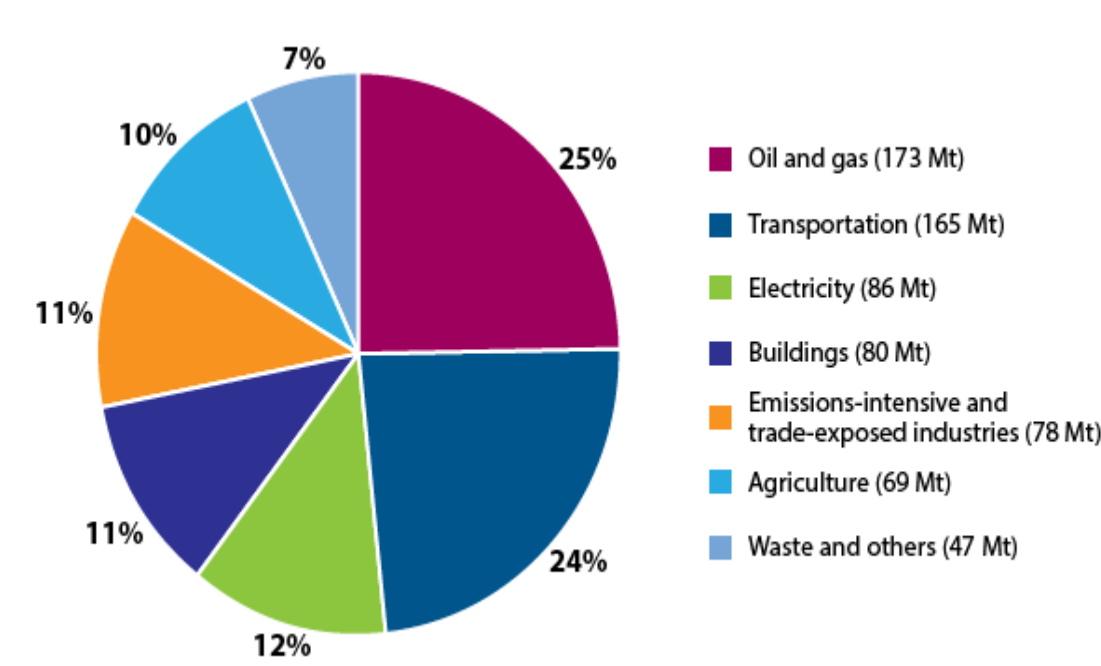


# Advanced Electrochemical System for Energy Storage Through CO<sub>2</sub> Conversion

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## BACKGROUND

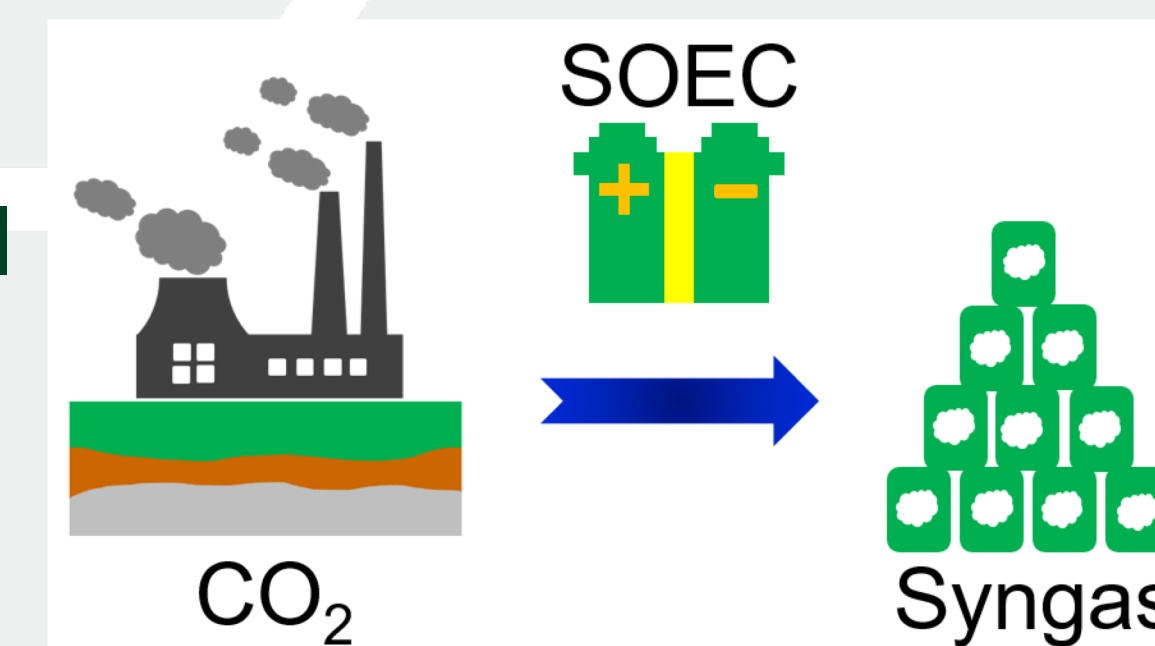
In Canada, over half of CO<sub>2</sub> emissions come from transportation or the oil and gas industry. Global warming is the result of enhancing the atmospheric greenhouse effect by the constant addition of greenhouse gases into the atmosphere from industrial emissions.



**CO<sub>2</sub> utilization: One of the best options for the future of green technology integration**

## AIMS AND OBJECTIVES

- Development of a stable, high performing solid oxide electrolysis cell (SOEC) that demonstrates tunable syngas production from CO<sub>2</sub> and steam at the cathode, and a pure O<sub>2</sub> stream at the anode, while also serving to store renewable and excess grid electricity.
- Exploration of the mechanism of CO<sub>2</sub> adsorption and activation on the surface of catalysts by using DFT calculation.



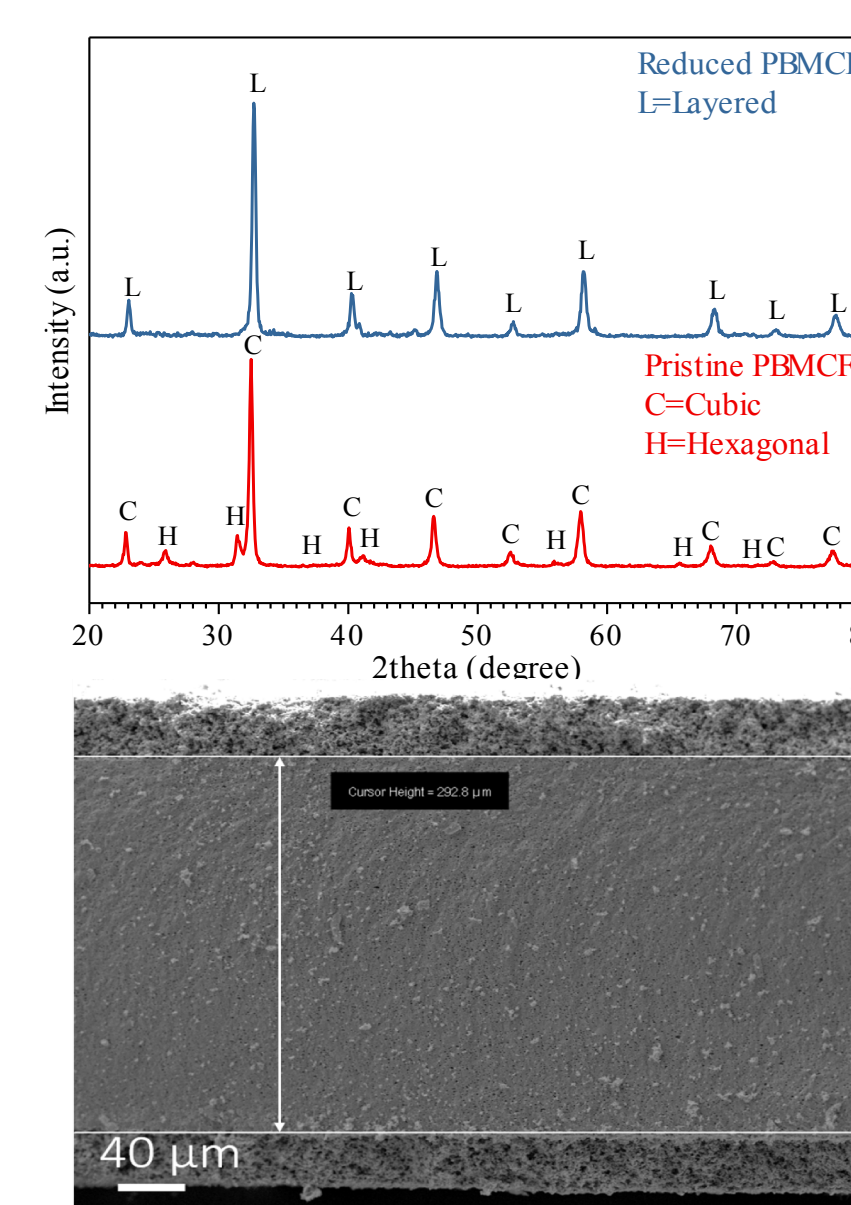
## RESULTS

### Catalyst for CO<sub>2</sub> conversion and cell fabrication

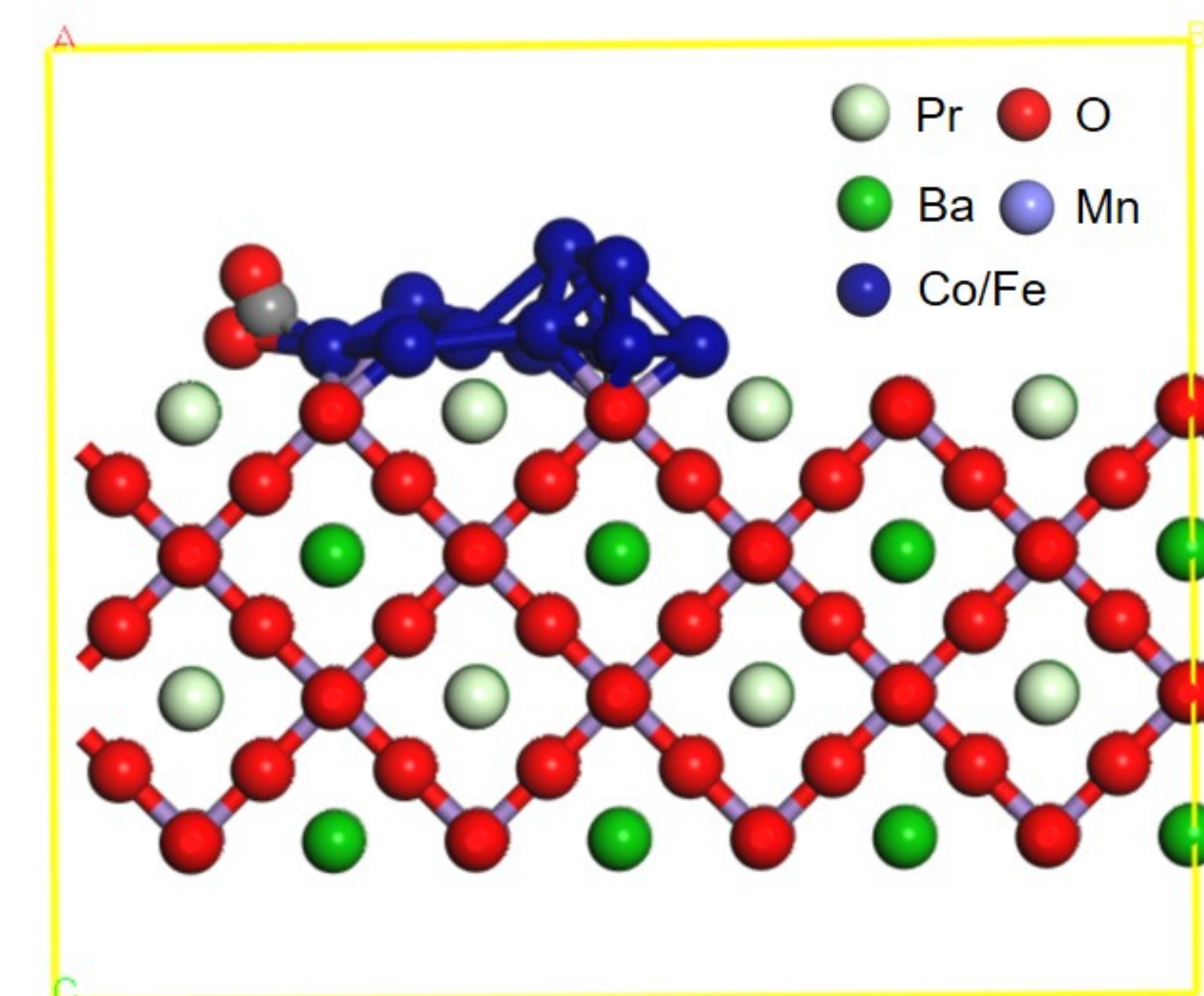
- **Catalyst Selection:** Co and Fe co-doped Pr<sub>0.5</sub>Ba<sub>0.5</sub>MnO<sub>3</sub> (PBMCF)
  - The phase of PBMCF will transfer from simple perovskite into layered double perovskite under reduction conditions.
  - Doped Co and Fe will exsolve under reduction conditions and form CoFe alloy nanoparticles on the catalyst surface.
- **SOEC Fabrication:** YSZ electrolyte supported cell

### Density functional theory (DFT) simulation

- **Crystal Structure Optimization**
  - Create and optimize the PBMCF models before and after reduction.
  - Investigate the energy change of phase transition.
- **Chemical adsorption/activation of CO<sub>2</sub> on the catalyst surface**
  - Create and optimize the adsorption model.
  - Investigate the CO<sub>2</sub> adsorption sites on the catalyst surface.



(Top) X-ray diffraction patterns of PBMCF before and after reduction.  
(Bottom) SEM image of YSZ supported SOEC.



Schematic image of adsorption configuration of CO<sub>2</sub> on PBMCF surface

## FUTURE DIRECTIONS

### Performance improvement

- Optimize the doping amount of Co and Fe.
- Optimize the microstructure of SOEC cell.
- Investigate the interface between PBMCF perovskite and the exsolved CoFe alloy nanoparticles.

### Theoretic investigation

- Density of states (DOS) and bandstructures of PBMCF perovskite before and after phase transition.
- Charge density difference of PBMCF with exsolved CoFe alloy nanoparticles on its surface.

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## FES PROJECT OVERVIEW

Hydrocarbons will continue to serve as an essential energy source while the world transitions to a lower-carbon energy economy, but can we prevent the use of those fuels from contributing to the accumulation of CO<sub>2</sub> in the atmosphere? Existing technologies can capture carbon, but these methods can be costly and energy-intensive. Extracting energy without burning fuels, improving CO<sub>2</sub> capture efficiencies if they are burned, and finding effective ways to store or reuse captured carbon may be essential to ensuring it does not enter the atmosphere.