The University Of Sheffield.
Chemical & Biological Engineering
Engineering at Sheffield.
Phebe L. Bonilla Prado
PhD Student
University of Sheffield
plbonillaprado1@sheffield.ac.uk
Prof Meihong Wang
Supervisor
University of Sheffield
Grantham Centre for Sustainable Futures
CONACYT
Consejo Nacional de Ciencia y Tecnología

Molecular simulation of CO_2 capture on Hydrotalcites as Solid Adsorbents

Introduction

- Carbon Capture, Utilization and Storage technologies CCUS, will play a crucial role in the future. However, their current cost is high.

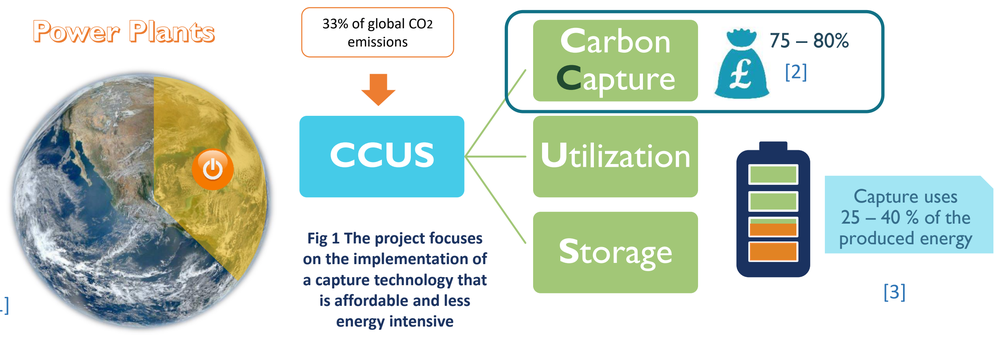

Fig 1 The project focuses on the implementation of a capture technology that is affordable and less energy intensive

- The implementation of solid adsorption could reduce the cost of carbon capture and favor CCUS widespread.
- Molecular can be used as tools to reduce the amount of resources and time spent on characterization studies of solid adsorbents. The information obtained can then be transferred to process simulations in order to scale up the results, without the need of building a pilot plant.

Objective

To develop a molecular simulation that predicts the adsorption capacity of hydrotalcites.

Solid Adsorption

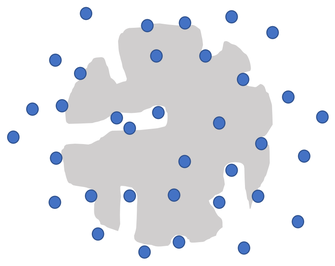

Fig 2 Adsorption process.

Solid adsorption is an exothermic and spontaneous process where particles or molecules get attached to the surface of a solid material, the **adsorbent.** Among the carbon-capture existing technologies, such as liquid absorption (commercially available), membranes and cryogenic distillation, **solid adsorption** has several advantages [4]:

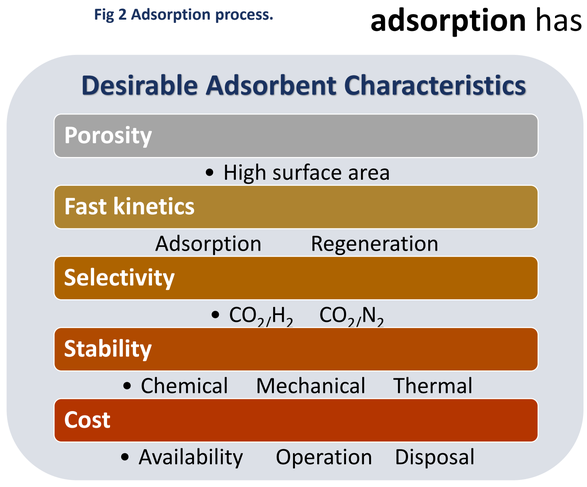

Fig 3 Desirable adsorbent characteristics.

- Lower energy requirements
- Lower installation and operation costs
- Useful in a wide range of temperature (40-500°C) and pressure (1 – 40 bar)
- No need of specialized waste treatment

[5]

Hydrotalcites HT

- HT are a type of anionic clay successfully used for CO2 adsorption at laboratory scale.
- Are widely available and are easy to synthesize.
  - Calcination of the HT is necessary to increase its adsorption capacity
- HT have relatively low adsorption capacity, which can be improved depending on:
  - Elements that integrate the HT
  - Conditions of synthesis and operation. [6]

$$\left[M^{+2}_{(1-x)}M^{+3}_{x}(OH)_2\right]^{+x}\left[\frac{A^{-n}_{x}}{n}\cdot yH_2O\right]^{-x}$$

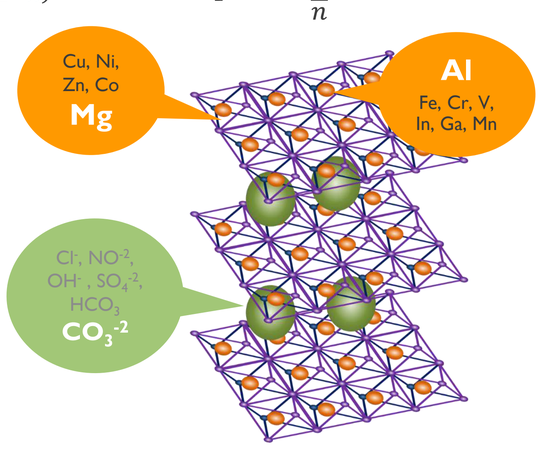

Fig 4 Hydrotalcite chemical formula and structure, with eligible elements.

Molecular Simulation Methodology

1. **ReaxFF Force Field Generation**: **ReaxFF** is a computational method that emulates chemical reactions. To do so, it needs adequate initial parameters set in the Force Field. ReaxFF then calculates the total energy of the system.

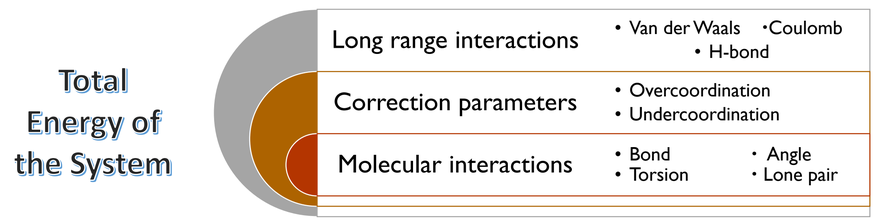

Fig 5 Energies calculated with the ReaxFF method to obtain the total energy of the system.

2. **Validation**: Molecular simulations carried out with **ADF Software** must be compared against literature and experimental results to assess the accuracy of the adsorption capacity prediction.
3. **Analysis**: Once the model is appropriate, the pressure and temperature parameters will be optimized to improve the adsorption capacity of HT.
4. **Process simulation**: The hydrotalcites obtained information will be used in scaled-up process simulations to further analyze their applications.

The project is in the first stage. The specialized force field for hydrotalcites in ReaxFF method has been developed and is under reparametrization using a Monte Carlo algorithm.

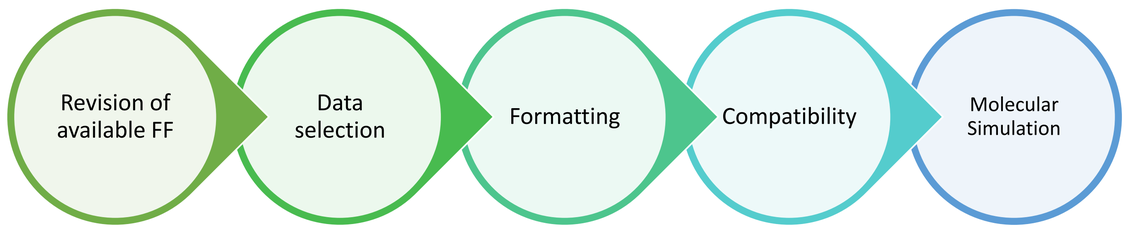

Fig 6 Stages of the FF development.

Results

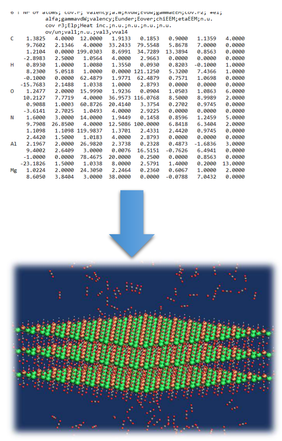

Fig 7 Screenshot of the developed FF and of the simulation using the modified structure of hydrotalcite.

Force Field

- A ReaxFF FF has been developed for hydrotalcite (Mg^{+2} and Al^{+3} as cations and CO_3^- as anions)
- The FF was coupled with a modified crystallographic structure based on the 82874.cif from the ICSD.

Simulation

- Preliminary results of the simulation show the total energy is stable after 500 iterations.
- After the simulation is completed, the FF will be reparametrized using a Monte Carlo algorithm.

Conclusions

- CCUS technologies are essential for reducing our CO_2 emissions.
- **Hydrotalcites** as solid **adsorbents** for CO_2 capture are a promising material which can be used in different operation environments
- **Molecular simulation** is a useful tool to provide insights of
  - Reaction mechanisms
  - Physical phenomena
- The quality of the simulation depends on:
  - Computational power
  - Theoretical model used
  - Initial **parameters**
- Future work includes the **reparameterization** of the current force field and simulations in for different ranges of pressure and temperature.

References

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