Motivation

- Due to the environmental issues that the world faces today, there are significant interests to develop materials capable to capture CO₂ with optimal performances.
- Solid materials are potential candidates for CO₂ sorbents. By combining the database mining with ab initio thermodynamic calculation, we implemented a novel theoretical methodology to screen solid sorbents from known material database and to synthesize new materials with improved CO₂ capture capabilities for further experimental validations.

Thermodynamic Properties of Capture Reaction

Heat of Reaction
- Van’t Hoff Plot
- Δμ-T-P Relationships

High-Throughput Screening Methodology

- Solids Bank
- Perform theoretical modeling.
- Search databases to find new thermodynamic properties.
- Screen sorbents using algorithms & QSPR.
- Perform experiments to validate screening.

Application to Alkali and Alkaline Metal Materials

- MF, NO, MOCO, MICO, MNO, MNI, MgCO, NaMgCO
- Search databases to find new thermodynamic properties.
- Screen sorbents using algorithms & QSPR.
- Perform experiments to validate screening.

Theoretical Methods

For the reaction of a solid to absorb CO₂ (s) are optional):

\[
solid_{sorbent} + CO_2 + [H_2O] \rightarrow solid_{CO_2} + [solid]
\]

The chemical potential (Δµ) of the reaction can be calculated as:

\[
\Delta \mu (T, P) = \Delta \mu^0 (T) - RT \ln(P_{CO_2} + P_{H_2O}/K_{H_2O})
\]

A. Intensive search for thermodynamic properties of solids from known databases and literatures. If all of them are known, obtain the better candidates by minimizing free energies based on operating conditions.
B. If their thermodynamic properties are unknown, calculate by

\[
\Delta \mu^0 (T) = \Delta \mu^0 (T) + T \Delta S (T) - T \Delta H (T)\]

Reactions Heat:
- \( \Delta H_{T, P}^0 \) calculated by density functional theory.
- \( \Delta S_{T, P}^0 \) calculated by thermochemical equations.

Phase-diagram

III. Doped Solid Materials to Adjust Turn-On Tᵯ

- \( \Delta \mu (T) \) calculated by density functional theory.
- \( \Delta S_{T, P}^0 \) calculated by thermochemical equations.

Conclusions

- Our theoretical approach can obtain similar results as experimental measurements and can be used to identify better candidates.
- The strength of our method is to screen complex sorbent materials for which their thermodynamic properties are not available.
- Hundreds of solid materials have been investigated. Now, we are working on screening of multi-components, substituted, doped, and mixed materials to search for good CO₂ sorbents.
- By mixing/doping different solids, we can theoretically synthesize new materials which may fit the industrial operating conditions with optimal CO₂ capture performance.
- As a long time goal, we’ll build a database of solid sorbents for CO₂ capture to satisfy industrial operational requirements.

Synthesis New Sorbents to Fit Operation Needs

I. Mixture A/B Sorbents (T> Tᵯ) using A capture CO₂ by decreasing Tᵯ

- By mixing A/B solids (diff) into Li₂SO₃ to form lithium silicates (micromerites), the free energy T of the newly formed material is lower than Tᵯ.
- By adjusting ratio of A and B, the Tᵯ could be shifted into the range which is a particular CO₂ capture technology needs.

Acknowledgement


Publications


References:


Acknowledgement