Computational Designing and Screening of Solid Materials for CO₂ Capture

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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 databases and to synthesize new materials with improved CO₂ capture capabilities for further experimental validations.

Theoretical Methods

For the reaction of a solid to absorb CO₂([...]) are optional):

\[ \text{solid}_\text{soberent} + \text{CO}_2 + [\text{H}_2\text{O}] \rightarrow \text{solid}_\text{soberent}_\text{CO}_2 + [\text{solid}] \]

The chemical potential (\(\Delta\mu\)) of the reaction can be calculated as:

\[ \Delta\mu(T,P) = \Delta\mu(T) - RT \ln P_{\text{CO}_2} \]

- If the thermodynamic properties of solids are known, calculate by
- If their thermodynamic properties are unknown, calculate by

\[ \Delta\mu(T) = \Delta\mu^\text{ent}(T) + \Delta\mu^\text{entr}(T) + \Delta\mu^\text{gibb}(T) + \Delta\mu^\text{chem}(T) \]

\[ \Delta\mu^\text{ent}(T) = \Delta H_{\text{fus}} + \Delta H_{\text{vap}} \]

Heat of Reaction

Van’t Hoff Plot

\[ T = \frac{-\Delta\mu^\text{f}(P)}{R \ln P_{\text{CO}_2}} \]

\[ \Delta\mu(T,P) = \Delta\mu(T) - RT \ln P_{\text{CO}_2} \]

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.

Publications


Acknowledgement