First Principles-based Computational Design of Novel High-Efficiency Solvents for Carbon Dioxide Capture

Gyeong S. Hwang

gshwang@che.utexas.edu

UTA

Research Goals

- This proposal intends to provide a theoretical foundation for the rational design and synthesis of novel sorbent materials for CO2 capture that are more energy efficient with higher capture capacity and faster absorption/desorption rates, in comparison to conventional solvents.

Research Contents

- Developing a robust computational platform capable of quantitatively evaluating the CO2 capture capacity of various sorbents of interest, based on a detailed understanding of the atomistic mechanisms governing the absorption and desorption of CO2 as well as the thermodynamic and dynamic properties of chosen sorbents.
- This proposed research exploits recent significant advances and harnesses the synergism possible by seamlessly coupling various state-of-the-art computational methods that range from quantum chemistry, molecular mechanics, to statistical theories.
- We anticipate that the outcome will provide valuable hints on how to improve the performance of existing solvents and how to design and synthesize energy and cost-efficient new materials by tuning functional groups and additives.

Expected Effects

- The systematic and integrated computational approach will greatly assist in achieving an improved understanding of CO2 capture/ regeneration phenomena and the involved mechanisms and chemistry, while current experimental techniques alone are limited to providing complementary real space information.
- The outcome will further provide valuable hints on how to improve the performance of existing solvents and how to design and synthesize energy and cost-efficient solvent materials.
- Furthermore, while the proposed theoretical research plans to be conducted in close collaboration with the existing KCCS experimental effort, we anticipated that having the experiments look to the theory and the theorists look to the experiments for feedback and direction leads to the type of cross fertilization that can produce unexpected breakthroughs.