

# CO<sub>2</sub> Molecular Basket as High-Capacity Adsorbent for CO<sub>2</sub> Capture from Flue Gas of Fossil Fuels-Based Electric Power Plants

## Goal

The goal is to develop a nano-porous solid adsorbent for CO<sub>2</sub>, which can be used as a molecular basket for CO<sub>2</sub> in condensed form. This can lead to development of high-capacity solid adsorbent for effective capture and separation of CO<sub>2</sub> from flue gas of fossil fuel-based power plants without the need for pre-separation of moisture or oxygen.

## Team

The Energy Institute is working with several organizations on the development of molecular basket for CO<sub>2</sub> capture. A partial listing includes: U.S. Department of Energy (DOE), National Energy Technology Laboratory, and U.S. Department of Defense (DOD).

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College of Earth & Mineral Sciences • Penn State University

## Background

The increased concentration of CO<sub>2</sub> in the atmosphere due to emissions of CO<sub>2</sub> from fossil fuel combustion has caused concern for global warming because CO<sub>2</sub> is a greenhouse gas. Adsorption is one of the promising methods that could be applicable for separating CO<sub>2</sub> from gas mixtures, and numerous studies have been conducted on separation of CO<sub>2</sub> by adsorption in the last two decades. Developing an adsorbent with high CO<sub>2</sub> selectivity and high CO<sub>2</sub> adsorption capacity, which can also be operated at relatively high temperature, is desired for more efficient CO<sub>2</sub> separation by adsorption method.

## Project Discussion

For practical application, selective adsorbents with high capacity are desired. A new concept called “molecular basket”, is proposed and explored in this project for developing high-capacity, highly-selective CO<sub>2</sub> adsorbent. In order to obtain high adsorption capacity, a large pore volume porous material should be used as the support material. In order to increase the affinity between the adsorbent and CO<sub>2</sub>, and further to increase the separation factor, a substance with numerous CO<sub>2</sub>-affinity sites should be loaded into the pores of the support. The objective of the work is to develop a nanoporous solid adsorbent, which can be used as a molecular basket for CO<sub>2</sub> in condensed form without the need for pre-separation of moisture or oxygen. Mesoporous molecular sieve MCM-41 with pore diameter of 3 nano-meter was hydrothermally synthesized. The polyethyleneimine (PEI) modified MCM-41 was prepared by wet impregnation method. The adsorption and desorption performance of the adsorbent was measured using a PE-TGA 7 analyzer, and further studied by using a flow apparatus with on-line gas chromatograph.

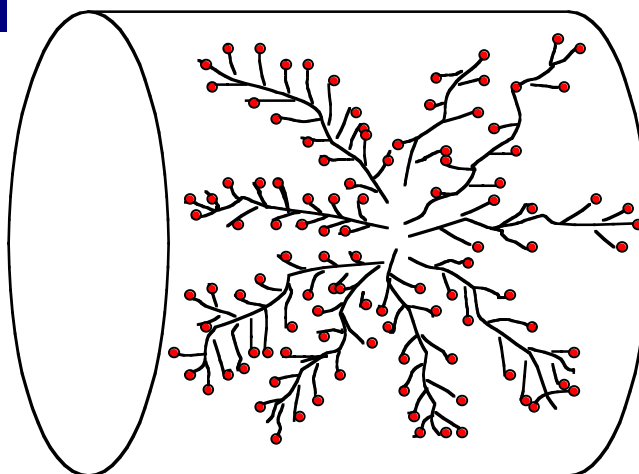


Figure 1: Concept of CO<sub>2</sub> Molecular Basket. Red dots indicate CO<sub>2</sub>-capturing sites in the “molecular basket”.

## Results

The physical properties of the adsorbents were characterized by X-ray powder diffraction (XRD), N<sub>2</sub> adsorption/desorption and thermogravimetric analysis (TGA). The characterization indicated that the structure of the MCM-41 was preserved after loading the PEI and the PEI was uniformly dispersed into the channels of the molecular sieve. The adsorption and desorption performance of the MCM-41-PEI-50 at different temperature in pure CO<sub>2</sub> atmosphere were measured. Figure 2 shows the synergetic effect of using MCM-41 and polymer PEI for CO<sub>2</sub> adsorption. The use of MCM-41 showed a synergetic effect on the adsorption of CO<sub>2</sub> by PEI. By loading the PEI into the MCM-41 pore channels, the adsorption capacity of the MCM-41 was significantly increased. Further, the desorption rate of CO<sub>2</sub> for MCM-41-PEI was faster than that for pure PEI.

Novel CO<sub>2</sub> “molecular basket” based on PEI modified mesoporous molecular sieve of MCM-41 (MCM-41-PEI) has been successfully developed. The novel “molecular basket” concept used resulted in a CO<sub>2</sub> adsorption capacity of 133 mg/g-adsorbent, which was 15.5 times higher than that of the MCM-41 and about 2 times higher than that of pure PEI.

In addition, the mesoporous MCM-41 molecular sieve support showed a synergetic effect on the adsorption of CO<sub>2</sub> when loading it with PEI, and also there was a significant decrease in the desorption time needed for recycling the adsorbent. The novel “molecular basket” material can effectively adsorb CO<sub>2</sub> at very low CO<sub>2</sub> concentration, e.g., 0.5%, and it is stable in cyclical operations at relatively high temperatures.

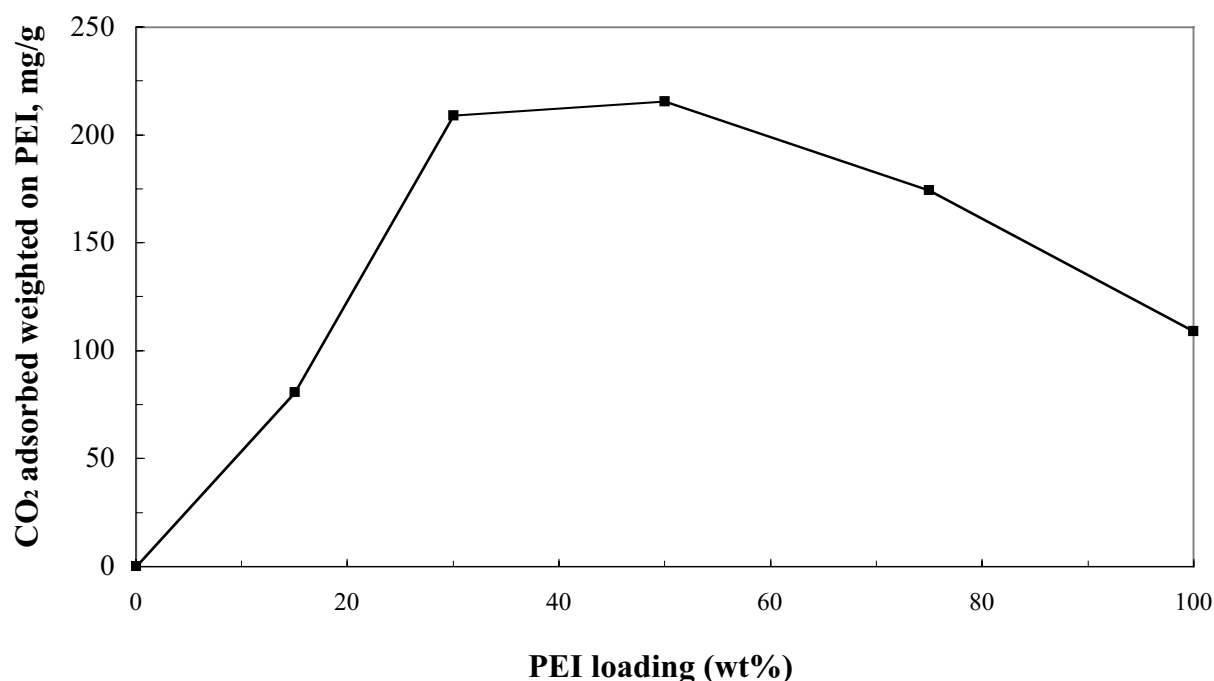


Figure 2: CO<sub>2</sub> Adsorption Capacity Weighted on Polymer PEI Loaded in MCM-41-PEI Adsorbent

### Key Publications

X. Xu, J. M. Andrésen, C. Song, B. Miller and A. W. Scaroni. Novel Polyethylenimine-Modified Mesoporous Molecular Sieve of MCM-41 Type as Adsorbent for CO<sub>2</sub> Capture. *Energy & Fuels*, to be published, 2002.

X. Xu, J. M. Andrésen, C. Song, B. Miller and A. W. Scaroni. Preparation of Novel CO<sub>2</sub> Molecular Basket” of Polymer-Modified MCM-41. *Am. Chem. Soc. Div. Fuel Chem. Prep.*, 2002, 47 (1), 67-68.

X. Xu, J. M. Andrésen, C. Song, B. Miller and A. W. Scaroni. Novel Adsorbent for CO<sub>2</sub> Capture Based on Polymer-Modified Mesoporous Molecular Sieve of MCM-41 Type. Abstract accepted for oral presentation, and manuscript to be submitted for publication in the Proceedings of 18th International Pittsburgh Coal Conference, Newcastle, NSW, Australia, December 3-7, 2001, Paper No. 17-2.