Computational Carbon Capture

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Carbon Capture and Sequestration

**EXPLANATION**

- **CO₂ injection**
- **Enhanced fossil-fuel recovery**
- **Conventional fossil-fuel recovery**
Decadal Land–Surface Average Temperature

10–year moving average of surface temperature over land
Gray band indicates 95% uncertainty interval
Decadal Land–Surface Average Temperature

10-year moving average of surface temperature over land
Gray band indicates 95% uncertainty interval

Temperature Anomaly (°C)

Oct 2012

Sea Ice Concentration Anomalies

(A) Surface air temperature anomaly north of 65°N

(B) Anomaly of sea ice extent (NH)

(C) Anomaly of frozen ground extent (NH)

(D) Anomaly of snow cover extent (NH)

Year


Sea Level Anomalies (mm)


Total anomaly = 0.3 million sq km

2004

Thursday, June 12, 14
Consequences:
velocity of climate change

- Historic rates: fastest 1 km/yr
- 28% of the surface > 1 km/yr

**Figure 2.5.11** The velocity of climate change
*Figure by Loarie et al. (2009)*
Figure 1.2.1 World energy consumption
U.S. Primary Energy Consumption Estimates by Source, 1850-2010

Source: U.S. Energy Information Administration Annual Energy Review, Tables 1.3, 10.1, and E1
“plan B”?  

Solving the climate problem for the next 50 years with current technologies

S. Pacala and R. Socolow,  
*Stabilization wedges: Solving the climate problem for the next 50 years with current technologies*  
Increase fuel economy of two billion cars from 30 to 60 mpg

Drive two billion cars not 10,000 but 5,000 miles a year (at 30 mpg)

Cut electricity use in homes, offices, and stores by 25%

Raise efficiency at 1,600 large coal-fired plants from 4- to 60%

Replace 1,400 large coal-fired plans with gas-fired plants

Install CCS at 800 large coal-fired plants

Install CCS at coal plants that produce hydrogen for 1.5 billion vehicles

Install CCS at coal-to-syngas plants

Install CCS at coal-to-nuclear plants to displace coal

Add twice today’s nuclear output to displace coal

Increase wind power 80-fold to make hydrogen for cars

Increase wind power 700-fold to displace coal

Increase solar power 700-fold to displace coal

Increase wind power 80-fold to displace coal

Source: Socolow and Pacala

Scientific American 2006
Different wedges

1000 Gigatons CO₂
(ramp up from 1 Gt/yr to 15 Gt/yr)
What to do with a GIGATON of CO$_2$?

Let’s convert CO$_2$ into “Dreamium™”
(in Berkeley we recycle everything!)

www.TwentyThousandMinusThreeAppsOfDreamium.com

Abhoyjit S. Bhown (EPRI):
<table>
<thead>
<tr>
<th></th>
<th>Estimated USA production</th>
<th>Estimated global production</th>
</tr>
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<tr>
<td></td>
<td>Mt</td>
<td>Gmol</td>
</tr>
<tr>
<td>1</td>
<td>Sulfuric acid</td>
<td>38.7</td>
</tr>
<tr>
<td>2</td>
<td>Nitrogen</td>
<td>32.5</td>
</tr>
<tr>
<td>3</td>
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<tr>
<td>4</td>
<td>Oxygen</td>
<td>23.3</td>
</tr>
<tr>
<td>5</td>
<td>Lime</td>
<td>19.4</td>
</tr>
<tr>
<td>6</td>
<td>Polyethylene</td>
<td>17.0</td>
</tr>
<tr>
<td>7</td>
<td>Propylene</td>
<td>15.3</td>
</tr>
<tr>
<td>8</td>
<td>Ammonia</td>
<td>13.9</td>
</tr>
<tr>
<td>9</td>
<td>Chlorine</td>
<td>12.0</td>
</tr>
<tr>
<td>10</td>
<td>Phosphoric acid</td>
<td>11.4</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>50</td>
<td>Nylon</td>
<td>1.9</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td><strong>419</strong></td>
<td><strong>8,681</strong></td>
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<tr>
<td><strong>2009 coal-fired generation GWe-yr</strong></td>
<td><strong>200</strong></td>
<td><strong>&gt;1000</strong></td>
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<tr>
<td><strong>Approximate CO₂ emissions</strong></td>
<td><strong>6,000</strong></td>
<td><strong>136,000</strong></td>
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</table>

Table 1.3.1 Comparison of CO₂ production and the production of chemicals
Figure 1.2.8 Distribution of (European) CO₂ emissions from different sources.
Carbon Capture and Sequestration

EXPLANATION

- CO₂ injection
- Enhanced fossil-fuel recovery
- Conventional fossil-fuel recovery
Figure 8.2.1 Injecting CO$_2$ below a caprock formation
(Figure based on information provided by CO2CRC)
Figure 8.2.2 Mechanisms of CO$_2$ trapping
Figure 8.2.2 Mechanisms of CO$_2$ trapping
(a) Stratigraphic trapping
**Figure 8.2.2** Mechanisms of CO$_2$ trapping
(b) Residual trapping
**Movie 8.2.1** CO₂ residual trapping simulation

*Movie from the CRC for Greenhouse Gas Technologies (CO2CRC)*

Introduction to Carbon Capture and Sequestration © 2014 by Imperial College Press
Figure 8.2.2 Mechanisms of CO$_2$ trapping
(c) Solubility trapping
Figure 8.2.2 Mechanisms of CO$_2$ trapping
(d) Mineral trapping
Figure 8.2.3 Trapping mechanisms as a function of time
(Figure adapted from Benson and Cole)
Figure 4.1.2 Coal-fired power plant with post-combustion carbon capture
**Box 4.1.2 Oxycombustion (Pre-combustion carbon capture)**

Cryogenic ASU

PC Boiler

Coal → heat recovery → NO\textsubscript{x} removal → PM/Hg removal → SO\textsubscript{x} removal → Compression → CO\textsubscript{2} storage

Steam → Steam Turbine → Electric Power

Recycle Compressor

Fans → water
Stage of CCS component technologies

<table>
<thead>
<tr>
<th>Stage of development</th>
<th>Concept</th>
<th>Lab testing</th>
<th>Demonstration</th>
<th>Commercial refinements needed</th>
<th>Commercial</th>
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<tbody>
<tr>
<td></td>
<td>Membranes</td>
<td>Chemical looping</td>
<td>Potential future breakthrough technologies</td>
<td>First projects are coming online now</td>
<td>Component technologies are mature; integrated platform to be proven</td>
</tr>
<tr>
<td></td>
<td>Oxy-fuel</td>
<td>Post-combustion</td>
<td>Pre-combustion</td>
<td>CO₂-EOR</td>
<td>CO₂-EOR</td>
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<tr>
<td></td>
<td>CO₂-EGR</td>
<td>Saline aquifers</td>
<td>Depleted oil and gas fields</td>
<td>Transport off-shore</td>
<td>Transport on-shore</td>
</tr>
<tr>
<td></td>
<td>Sleipner (Norway) field has been operational for around 10 years</td>
<td>Have been used for seasonal gas storage for decades</td>
<td>US has existing CO₂ pipeline network of more than 5000 kilometers</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Source: Interviews; Team analysis

Amines

in water:

\[ 2 \text{HO-}\text{NH}_2 + \text{CO} \leftrightarrow \text{HO-}\text{NH-}\text{COO}^- + \text{NH}_3 \]

• Large amounts of pure water required

• \(~30\%\) energy penalty for regeneration

Flue gas:
- 0.7 bar N\(_2\)
- 0.1 bar CO\(_2\)
More on CCS

iBook version

Carbon Capture

In the coming Control Age, scientists will be able to design and create entirely new materials and processes with desired properties and outcomes. With such capabilities, we should find solutions to some of the most vexing problems that civilization now faces, including energy, in all of its aspects, and changing global climate patterns.

EFRC - Carbon Capture

Capture of CO₂ from gas mixtures requires the molecular control offered by nanoscience to tailor-make those materials exhibiting exactly the right adsorption and diffusion selectivity to enable an economic separation process. Characterization methods and computational tools will be developed to guide and support this quest.
Carbon Capture and Sequestration Research

Capture is currently considered to be the most expensive part of CCS.

Geologic storage involves uncertainties and risks when considered at full scale.
Gas separations

Important CO₂ separations:

• Flue gasses (coal 12% CO₂; natural gas 4% CO₂)
  • “End of pipe” technology; low pressure

• Natural gas
  • High pressure form natural reservoirs

• CO₂ directly from air
  • Ultra low concentration of CO₂

• Oxygen from air:
  • Oxy-combustion
Solid Adsorbents
- Jeffrey Long (UC Berkeley)
- Omar Yaghi (UC Berkeley)
- Hong-Cai Zhou (Texas A&M)

Polymer Membranes:
- Frantisek Svec and Jean Frechet (LBNL)
- Bret Helm and Ting Xu (LBNL)
- Dave Luebke (NETL)

Characterization
- Resonance soft X-rays: Blandine Jerome and Jeff Kortright (LBNL)
- X-ray crystallography: Simon Teat (LBNL)
- NMR: Jeffrey Reimer (UC Berkeley)

Computation
- Adsorption and Diffusion: Berend Smit (UC Berkeley)
- Electronic Structure calculation: Jeff Neaton (LBNL) and Gullia Galli (UC Davis)
- Quantum calculations: Laura Gagliardi (U Minnesota)
- Materials Screening: Maciej Haranczyk (LBNL)
Metal Organic Frameworks

- BET surface areas up to 6200 m²/g
- Density as low as 0.22 g/cm³
- Tunable pore sizes up to 5 nm
- Channels connected in 1-, 2-, or 3-D
- Internal surface can be functionalized
- BASF production on ton scale

\[ \text{Zn}_4\text{O}(1,4\text{-benzenedicarboxylate})_3 \]

MOF-5
Computation Challenge

Chemical Flexibility of MOFs

- We can change the metal: Fe, Mg, Ca, Zn, Cu, etc
- We can change the linker
- We can change the pore topology

Out of these many many millions of structures, which one is the best for Carbon Capture?
How to compare two MOFs

My MOF has the highest selectivity

My MOF the has the largest pore volume
Separating CO$_2$

$\text{CO}_2/\text{N}_2$ $\xrightarrow{\text{adsorption}}$ N$_2$

$\text{loading}$ $\uparrow$

$\text{CO}_2$ $\xrightarrow{\text{desorption}}$ N$_2$

$\text{Partial pressure}$

Thursday, June 12, 14
Working capacity & Henry coefficient

- **Slope**: Henry coefficient
- **Flue gas at 40°C**
- **Desorption $T$**
- **Working capacity**

Loading vs. Partial pressure graph with points at 0.15 atm and 1.0 atm.
Increasing the working capacity: temperature

Flue gas at 40°C

desorption $T_d$

$T \ll T_d$

loading

Partial pressure

0.15 atm

1.0 atm
Increasing the working capacity: **pressure**

We can increase the working capacity, but at which cost?
Model for Screening Materials

Calculate *process independent performance* characteristics of materials for CCS

- Fixed bed configuration
  - Temperature swing
  - Pressure swing
  - Hybrid processes
- Equilibrium model
  - No heat or mass transfer
  - Based on isotherms
- Uses difference in capacity between *adsorption / desorption* conditions

(Adam Berger and Abhoyit Bhow, EPRI)
Performance metric: parasitic energy

Energy penalty for Carbon Capture and Sequestration:

**compression work** and the **heating energy**:

- Heating energy (Q): heat necessary to regenerate a given sorbent:
  - Sensible heat: heats and cools bed. Provides driving force to produce CO\(_2\)
  - Desorption heat: desorbs CO\(_2\) (equal to heat of adsorption, \(\Delta h\)).

\[
Q = \left( C_p \rho_{sorbent} \Delta T + \Delta h_{CO_2} \Delta q_{CO_2} + \Delta h_{N_2} \Delta q_{N_2} \right) / CO_2\text{Produced}
\]

- Compressor work (\(W_{comp}\)): Work to compress CO\(_2\) to 150 bar (for transport)

\[
W_{eq} = \left( 0.75 Q \cdot \eta_{\text{carnot}} + W_{\text{comp}} \right)
\]

- Parasitic energy calculated by discounting the heat requirement by the Carnot efficiency to simulate the effect of taking steam from a steam cycle
• 180 Known structures
• >3,000,000 hypothetical structures
• **Which is the best for carbon capture?**
Zeolites for Carbon Capture

Equivalent Energy for those all silica structures with experimental data

What is the best structure?

What is the lowest energy?
Molecular Simulations

- Molecular dynamics: solve equations of motion
- Monte Carlo: importance sampling

→ calculate thermodynamic and transport properties for a given intermolecular potential
Zeolites (MFI)

Open: simulations
Closed: experiments

All known zeolites

Equivalent Energy (KJ/Kg CO\textsubscript{2})

\text{CO}_2\text{'}s Henry\text{'}s Law Coefficient (mol/Kg * Pa)
What is the best zeolite structure? (Materials Genome)

Hypothetical zeolites

\(~2.7 \times 10^6\) unique structures were enumerated, with roughly 10% within the +30 kJ/mol Si energetic band above R-quartz in which the known zeolites lie.

How to predict 1 million isotherms?

CPU: one isotherm 5-10 days

- Less than 20 cores
- Designed for general programming

GPU
trade-off between memory, # threads, and work load
• Energy calculation in parallel
• Monte Carlo in parallel for different pressures

- More than 500 cores
- Optimized for SIMD (same-instruction-multiple-data) problems

Screening: > 300,000 structures
Identified many structures with a significantly lower parasitic energy compared to the current technology

.... and now MOFs
Materials synthesized in EFRC represent a class of materials. These materials not only indicate different compositions, but also different pore shapes. The material order from the top left: MFI, PPN-6, ZIF-78, (bottom left) Mg-MOF-74, HMOF-992 and CaA.

**FIG. 5.** Selection of analyzed materials. The shown structures are representatives for each class of materials under investigation. Atoms and bonds are illustrated as ball and sticks. Color-code for the atoms: red: oxygen, yellow: silicon, grey: carbon, white: hydrogen, blue: nitrogen, green: magnesium, brown: zinc, orange: aluminium, cyan: calcium, and purple: sodium. Material order: a) MFI, b) PPN-6, c) ZIF-78, d) Mg-MOF-74, e) HMOF-992, and f) CaA.

**Figure 6.** Illustrates the characteristic plot showing the parasitic energies for coal flue gas as a function of the CO$_2$ Henry coefficient ($k_{CO_2}$) at 300K. The parasitic energy of the currently applied MEA technology for coal flue gas was estimated to be at 1060 kJ/kg [11] and is depicted as a black solid line. The black dashed line indicates the envelope line of the all-silica structures [11] for the coal flue gas composition. Details to the envelope line can be found in the supporting information. The envelope curve exhibits a broad parasitic...
and is depicted as a black solid line. The black dashed line indicates the envelope line of the all-silica structures \[11\] for the coal flue gas composition. Details to the envelope line can be found in the supporting information. The envelope curve exhibits a broad parasitic energy optimum in a higher Henry coefficient region. This significant region lies below MEA technology and highlights the pursued material property. Henry coefficients lower than \(10^{-4}\) mol/kg·Pa lead to higher parasitic energies due to the small accessible working capacity. Higher Henry coefficients (\(K_H, CO_2 > 10^{-2}\) mol/kg·Pa) yield a steep increase of the parasitic energy as the \(CO_2\) adsorption gets very strong and additional energy is needed to regenerate the material \[11\].

FIG. 6. Characteristic plot of parasitic energy for coal flue gas. Circles depict parasitic energy results for each material. Current MEA technology is marked as black solid line, black dashed line shows envelope for coal, and black dotted line indicates lowest predicted parasitic energy (Mg-MOF-74: 727.12 kJ/kg\(CO_2\)). Color code for material classes: cation exchanged zeolites: black, zeolitic imidazolate frameworks: red, hypothetical materials: green, metal-organic frameworks: dark blue, porous polymer networks: magenta and zeolites: light blue. Mg-MOF-74 could reduce CCS requirement in coal about 30% compared to MEA. All investigated materials can be found along the all-silica envelope line which denotes that the experimental materials exhibit a similar trend like the theoretical ones with some deviation.
Coal, natural gas, and air

The black solid line represents the current MEA technology. The black dashed line indicates the envelope line for coal, and the black dotted line shows the lowest predicted parasitic energy (Mg-MOF-74: 727.12 kJ/kg CO₂). Current MEA technology could reduce CCS requirement in coal by about 30% compared to MEA.

All investigated materials can be found along the all-silica envelope line, indicating a similar trend like the theoretical ones with some deviation.
the experimental materials exhibit a similar trend like the theoretical ones with some deviation. CCS requirement in coal about 30% compared to MEA.

DFT Binding geometry of a single CO$_2$ molecule adsorbed inside Mg-MOF-74. The figure represents the binding geometry computed by the neutron powder diffraction experiment at 20K by Queen et al. It is also important to note that the predicted DFT geometry, model 4, agrees very well with the experimental binding geometry.

Furthermore, the parasitic energy as the CO$_2$ capacity gets very strong and additional energy is needed to regenerate the material [11].

Henry coefficients lower than 10$^{-4}$ mol/l are set to d = 2.4 Angstrom. Black closed squares are the DFT reference energies and the open metal sites of the vector of Mg distance.

**Figure 5:** Comparison between the DFT and force field interaction energies as a function of the angle $\theta$. This angle gives the orientation of O=C=O with respect to the Mg coordination sites.

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**Image 1:** Figure 6: DFT Binding geometry of a single CO$_2$ molecule adsorbed inside Mg-MOF-74. The figure represents the binding geometry obtained from DFT calculations. Table 1 gives the orientation of O=C=O with respect to the Mg coordination sites.

**Image 2:** Figure 5: Comparison between the DFT and force field interaction energies as a function of the angle $\theta$. This angle gives the orientation of O=C=O with respect to the Mg coordination sites.

**Image 3:** Figure 6: Characteristic plot of parasitic energy for coal flue gas. Circles depict parasitic energy results for each material. Current MEA technology is marked as black solid line, black dashed line indicates the envelope line of lowest predicted parasitic energy optimum in a higher Henry coefficient region. This significant region lies below MEA technology and highlights the pursued material property. Henry coefficients lower than 10$^{-3}$ mol/l lead to higher parasitic energies due to the small accessible working line shows envelope for coal, and black dotted line indicates lowest predicted parasitic energy.
Figure 3: Comparison of the CO$_2$-framework interaction energies obtained from the DFT calculations with the ones computed from the UFF (open blue squares) and the DFT-derived force field (model 1, open red circles) for a set of 1200 CO$_2$ random configurations inside the accessible pore volume of Mg-MOF-74. The green-dashed line indicates perfect agreement between the energies computed by DFT and by force fields.

At this point, it is instructive to compare our new force field with the one we previously derived from MP2-cluster calculations. The predicted adsorption isotherms by this MP2 force field are in good agreement with the experimental data (see Figure 4).

However, if we compare the MP2 force field predictions for a set of random configurations with the DFT energies (see SI Figure S3), we observe that the MP2 force field cannot nicely predict the DFT energies computed in the periodic system. The energies of CO$_2$ configurations located near the center of the pores are systematically overestimated. In addition, the minimum energy configuration that is predicted by this force field has a correct energy, but gives a different orientation than the one predicted by DFT. DFT predicts that the minimum energy configuration of O=C=O has an angle of $\sim 80^\circ$ with respect to the axis parallel to the channel, whereas the corresponding angle predicted by MP2 force field is significantly smaller ($<60^\circ$). Predicting this angle correctly is significantly important to reproduce the NMR measured line shape induced by CO$_2$ dynamics (see next section). These results suggest that the previously adopted clusters may have been too small to capture the range of possible interactions in the extended structure.
Each step is discussed in details in the following sections.

We use CO$_2$ adsorbed in Mg-MOF-74 as case study.

Figure 1: Flow diagram of the proposed method to derive force field from periodic DFT calculations.

Structural optimization (DFT)

Atom-types identification

Approaching paths determination

Interaction energy calculations (DFT)

Energy decomposition

Force-field parameterization ($S_g$, Repulsion)

Classical molecular simulation (MC/MD)

Self-consistent parameterization loop

Rank #1

Determine order

2 variables will be fitted in each step

Converged?

Rank #2

...
Force Fields

Quantum calculations (MP2) + NEMO decomposition

with Laura Gagliardi (U Minnesota)

**Figure 3: Comparison of the CO$_2$ framework interaction energies obtained from the DFT calculations with the ones computed from the UFF (open blue squares) and the DFT-derived force field (model 1, open red circles) for a set of 1200 CO$_2$ random configurations inside the accessible pore volume of Mg-MOF-74. The green-dashed line indicates perfect agreement between the energies computed by DFT and by force fields.**

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1.6 kJ/mol

Isosteric heat (kJ/mol)

Loading (\# CO$_2$ / Mg site)

Simmons et al.
Mason et al.
Dietzel et al.
MP2-derived FF
Water isotherms?

Figure 12: Comparison between the experimental and simulated isotherms for $H_2O$ inside Mg-MOF-74 at 298 K. The experimental isotherms are shown by the open symbols. The closed red circles and blue upper triangles represent the computed isotherms with the UFF and the DFT-derived force field (model B), respectively.

Figure 12: (a) Comparison between the experimental and simulated isotherms for H$_2$O adsorption in MgMOF-74 at 298 K versus ZnMOF-74.

- DFT-derived force fields:
  - Mg-MOF-74
  - Zn-MOF-74

- Structures:
  - current MEA
  - zeolite line
  - MOFs
  - CoMOF74
  - MgMOF74
  - NiMOF74
  - ZnMOF74

Parasitic Energy (kJ/(kg CO$_2$)) vs. Henry Coefficient of CO$_2$ (mol/kg/Pa)
Water–CO$_2$

**Figure 14:** Binary mixture inside (a) Mg–MOF–74 and (b) Zn–MOF–74. Left y-axis: simulated binary mixture uptake of CO$_2$ (red closed circles) and H$_2$O (closed blue squares) as a function of H$_2$O mole fraction at total pressure of 0.15 bar and temperature of 313 K. Right y-axis: the reduction of CO$_2$ uptake (%) as a function of H$_2$O mole fraction. The definition of reduction is the ratio of CO$_2$ uptake under the mixture condition to the pure component CO$_2$ uptake at (P, T) = (0.15 bar, 313 K).

It is interesting to compare the effect of water on adsorption of CO$_2$ in Zn–MOF–74. Compared to the Mg–MOF–74, given that the binding strength of water is much weaker, Zn–MOF–74 is less sensitive to the presence of trace amounts of water vapor. Our calculations show that there is nearly no degradation in the CO$_2$ uptake before the occurrence of water condensation inside the Zn–MOF–74 (i.e., ~2%, see SI Figure S6).

**Concluding remarks:** In summary, we have developed a new method to derive accurate force fields from periodic DFT calculations. The characteristic of this method is that we only calculate DFT energies on specific paths that are most sensitive to their corresponding pair-wise interaction between approached pairs. Compared to methods that use genetic algorithms, this reduces the number of required ab initio calculations. In addition, we use an energy decomposition scheme in combination with a self-consistent optimization.
Conclusions

• Parasitic energy is a useful concept to rank materials
  • best material adsorption not to strong/not to weak
  • Natural gas: higher adsorption is better
• EFRC: we can tailor make the best adsorbent if flue gasses where mixtures of N\textsubscript{2}/CO\textsubscript{2}
• Open metal sites
  • Very interesting chemistry: conventional force fields do not work
  • Systematic methods to develop force fields
  • Effect of water
• Materials Genome:
  • Intelligence versus brute force ....
  • Screening for best materials: what can be obtained
Carbon Capture, Utilization & Storage

Defining the Frontiers

May 31 - June 5, 2015
Stonehill College
Easton, MA

Chair:
Berend Smit

Vice Chair:
Ah-Hyung (Alissa) Park

Application Deadline

Applications for this meeting must be submitted by May 3, 2015. Please apply early, as some meetings become oversubscribed (full) before this deadline. If the meeting is oversubscribed, it will be stated here. Note: Applications for oversubscribed meetings will only be considered by the Conference Chair if more seats become available due to cancellations.

The new Gordon Research Conference (GRC) on "Carbon Capture, Utilization and Storage" will create a new forum for discussion at the frontiers of carbon management research, including fundamental scientific studies of CO₂ interactions with novel materials for Carbon Capture, Utilization and Storage (CCUS) as well as science policy essential for the deployment of CCUS.
Buy the book!

Thanks!

- Jihan Kim, Li-Chiang Lin, Joe Swisher, Roberta Poloni, Adam Berger, Allison Dzubak, Richard Martin
- Jeff Long (UC Berkeley)
- Jeff Neaton (LBNL)
- Jeff Reimer (UC Berkeley)
- Maciej Haranczyk (LBNL)
- Mike Deem (Rice)
- Laura Gagliardi (U Minessota)
- Abhoyjit Bhown (EPRI)

Support:
- Basic Energy Sciences (Department of Energy)
- ARPA-e (Department of Energy)