EFRC: CENTER FOR GAS SEPARATIONS RELEVANT TO CLEAN ENERGY TECHNOLOGIES (CGS)

UPDATED: AUGUST 2016

AWARDS: $10.8M (August 2009 – July 2014); $12.0M (August 2014 – July 2018)

WEBSITES: http://science.energy.gov/bes/efrc/centers/cgs/; http://www.cchem.berkeley.edu/co2efrc/

TEAM: **University of California, Berkeley (Lead)**: Jeffrey Long (Director), Jeffrey Neaton, Jeffrey Reimer, Berend Smit (Deputy Director), Ting Xu, Omar Yaghi; **Lawrence Berkeley National Laboratory**: Brett Helms, Jeffrey Kortright, Maciej Haranczyk, David Prendergast, Simon Teat, Steve Whitelam; **National Energy Technology Laboratory**: David Hopkinson; **National Institute of Standards and Technology**: Craig Brown; **Texas A&M**: Hong-Cai Zhou; **University of Minnesota**: Laura Gagliardi, Michael Tsapatsis; **École Polytechnique Fédérale de Lausanne:** Wendy Queen

SCIENTIFIC MISSION AND APPROACH

The major aim of CGS is to design and tailor-make new materials for the efficient separation of industrially-relevant gases, which requires the ability to discriminate between their often subtle chemical and physical differences. Thus, CGS is also developing novel characterization and computational methods to guide understanding of the materials properties necessary for such separation specificity and efficiency. Given that industrial separations processes currently account for 10-15% of total global energy consumption, efforts to reduce these energy costs by employing more effective materials represent a vital pursuit towards lowering our overall energy usage. In particular, CGS is targeting novel adsorbents for CO_2 capture, the separation of O_2 from air and N_2 from methane, and for the shape-selective separation of hydrocarbons. CGS research focuses on three major goals:

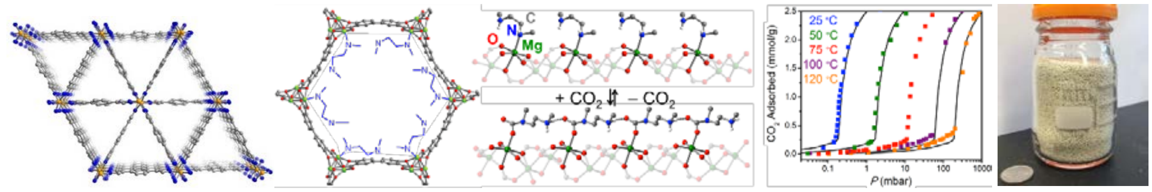
1) **Materials Synthesis:** Design and synthesis of new chemically and mechanically stable adsorbents for more energy-efficient gas separations.

2) **Materials Characterization**: Development of novel characterization tools for the rigorous understanding of adsorbent chemical and physical properties, including *in situ* characterization of gas binding in adsorbents via single-crystal X-ray diffraction, X-ray absorption, and nuclear magnetic resonance.

3) **Computational Separations**: Creation of novel computational methods to model gas adsorption behavior and to predict as-yet unknown adsorbents with promise in various separations applications.

SELECTED SCIENTIFIC ACCOMPLISHMENTS

- Discovered a new metal-organic framework (MOF), mmen-Mg_2(dobpdc), that exhibits remarkable CO_2 affinities and capacities arising from an unprecedented cooperative adsorption mechanism that enables material regeneration at much lower temperatures than currently used for amine solvents.
- Developed mixed-matrix (polymer and MOF) membranes that exhibit vastly improved separation of light hydrocarbons and resistance to plasticization relative to the pure polymers.
- Designed novel cobalt-based MOFs that exhibit selective and reversible binding of O_2 over N_2.
- Developed a new computational approach to evaluate a wide range of adsorbents on their performance for capture and storage of CO_2.
- Discovered MOFs that separate hydrocarbon mixtures found in gasoline or natural gas based on pore shape or exposed metal sites, paving the way for a less energy-intensive separation process than cryogenic distillation.
- Designed a highly versatile iron-based MOF that is capable of distinguishing small hydrocarbons as well as efficiently separating O_2 from N_2.



CGS research, from left: triangle channels separate hydrocarbon mixtures based on shape; diamine-appended MOFs can exhibit step-shaped isotherms arising from a new cooperative mechanism for CO_2 adsorption; Mosaic Materials is developing inexpensive methods to make tons of pelletized MOFs.

IMPACT

- Berend Smit and Jeff Reimer co-wrote a book, *Introduction to Carbon Capture and Sequestration*, which they have used to co-teach a University of California, Berkeley course. World Scientific Publishing recently highlighted the book as their best-selling text in energy studies.
- A short film about CGS, co-produced with World Energy TV, was broadcast at the 2016 World Future Energy Summit in Abu Dhabi. The summit is a major meeting for the advancement of clean and sustainable energy and draws over 30,000 attendees from business, academia, and industry. http://www.cchem.berkeley.edu/co2efrc/resources.html
- **Mosaic Materials, Inc.**, a start-up company co-founded by Jeffrey Long in June 2014, is working on large-scale synthesis and commercialization of diamine-appended MOFs for CO_2 capture from coal-fired power plants. The mmen-Mg_2(dobpdc) material was brought into an ARPA-E project that used high-throughput screening to identify optimal materials for the low-energy CO_2 capture. In this project, a material was discovered that can adsorb more than 10 weight % CO_2 at 25 °C and release the gas with heating to 80 °C, lowering the energy penalty for carbon capture from 30% for existing technology to an estimated 15% or less. The company is currently incubating within the Cyclotron Road program at Lawrence Berkeley National Laboratory. http://www.cyclotronroad.org/mosaic/
- **framergy, Inc.**, a small company started in 2011 to commercialize Hong-Cai Zhou's research, provides high-quality, high-volume MOFs, porous polymer networks, and ligands at low-cost for clean energy and other applications. IP created under CGS-funded research in the Zhou group is being licensed and developed by framergy. http://www.framergy.com/
- CGS research accomplishments have been the basis for over $500K in follow-on funding from ExxonMobil, Ishikawajima-Harima Heavy Industries (IHI), and the California Energy Commission.

PUBLICATIONS AND INTELLECTUAL PROPERTY

As of May 2016, CGS had published 214 peer-reviewed publications cited over 22,200 times, and filed 15 disclosures, 15 US patent applications, and 16 foreign patent applications. One patent has been issued and 12 patent applications licensed. The following is a selection of impactful papers:

- Bachman, J. E. *et al.* Enhanced Ethylene Separation and Plasticization Resistance in Polymer Membranes Incorporating Metal-Organic Framework Nanocrystals. *Nature Materials* **15**, 845-849, doi: 10.1038/nmat4621 (2016). [**4 citations**]
- McDonald, T. M. *et al*. Cooperative Insertion of CO_2 in Diamine-Appended Metal-Organic Frameworks. *Nature* **519**, 303-308, doi: 10.1038/nature14327 (2015). [**135 citations**]
- Kong, X. *et al.* Mapping of Functional Groups in Metal-Organic Frameworks. *Science* **341**, 882-885, doi: 10.1126/science.1238339 (2013). [**95 citations**]
- Sumida, K. *et al.* Carbon Dioxide Capture in Metal-Organic Frameworks. *Chemical Reviews* **112**, 724-781, doi: 10.1021/cr2003272 (2012). [**2132 citations**]
- Lin, L. C. *et al. In Silico* Screening of Carbon-Capture Materials. *Nature Materials* **11**, 633-641, doi: 10.1038/nmat3336 (2012). [**177 citations**]
- Bloch, E. D. *et al.* Hydrocarbon Separations in a Metal-Organic Framework with Open Iron(II) Coordination Sites. *Science* **335**, 1606-1610, doi: 10.1126/science.1217544 (2012). [**491 citations**]