Center for Gas Separations (CGS) EFRC Director: Jeffrey R. Long Lead Institution: University of California, Berkeley Class: 2009 – 2020

Mission Statement: To develop new materials and membranes that enable the energy-efficient separation of gas mixtures, as required in the clean use of fossil fuels and in reducing CO_2 emissions from industry.

Separation processes have been estimated to account for 10–15% of our total energy consumption. As the global population grows and our reliance on fossil fuels continues in the near term, this percentage is anticipated to increase significantly, both as raw material demand increases and as we make essential investment in large-scale carbon capture and sequestration technologies. Reducing the total energy costs associated with various separations in industry and powder generation would contribute significantly toward lowering our overall energy usage. The aim of the Center for Gas Separations (CGS) is to develop new porous materials that enable energy-efficient gas separations, based on unprecedented molecule-specific interactions, together with new and powerful characterization methods that provide a fundamental understanding of the properties and performance of such materials.

The challenge is to remove the fundamental scientific barriers that currently prohibit the energy-efficient separation of gases essential to the development of clean energy technologies. This challenge is significant, as the chemical and physical differences between molecules in gas mixtures of interest are often small, and therefore it is necessary, through the use of nanoscience and synthetic chemistry, to engineer unprecedented molecular-level control in adsorbate–adsorbent interactions and thereby tailor-make materials that have exactly the right adsorption and diffusion selectivity to enable an economic separation process.

The Center brings together personnel with expertise in the following areas:

- Materials Synthesis: The synthesis of new gas-permeable materials with control over the molecular functionalities is essential to enable preferential adsorption of gas molecules. Our focus here is on

 (i) generating novel metal–organic frameworks exhibiting molecule-specific chemical interactions and
 (ii) new membrane constructs incorporating these materials.
- Materials Characterization: Detailed atomic-level structural characterization of the new materials is
 necessary both before and after exposure to gas samples in order to probe interaction mechanisms
 and further tailor material properties. We develop novel characterization methods that enable us to
 accurately assess the selectivity, kinetics, and thermodynamics of gas adsorbate binding, both to
 demonstrate efficacy and test computational models.
- *Computational Separations*: A strong computational component to the research is essential for understanding chemical interactions at a molecular level, as well as for guiding the synthetic efforts toward materials exhibiting high specificity for a given adsorbate and tunable interaction energies.

We are developing exceptional new materials for a host of energy-related gas separations, including the separation of CO_2 from power plant flue streams, the separation of CO_2 from natural gas deposits, the separation of O_2 from air, the separation of N_2 from natural gas, and the separation of industrially relevant hydrocarbon mixtures.

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