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Gas separation using metal-organic framework membranes

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Abstract

In recent years, metal-organic frameworks (MOFs), a class of nanoporous materials, have received substantial attention due to their special adsorption properties for gas storage and separation. The separation of CO_2 from N_2 present in flue gas streams is especially significant due to the problems associated with CO_2 pollution of the atmosphere. Since gas separation is a combination of thermodynamic and kinetic processes, both adsorption and diffusion properties need to be taken into account. A huge challenge is that CO_2 and N_2 have similar kinetic diameters (CO_2 3.30 Å, N_2 3.64 Å), making the separation based purely on size very difficult. On the other hand, the modular nature of the MOFs makes them attractive for introducing specific functional groups which may enhance adsorption selectivity. Additional challenges are due to the chemical and thermal stability of the framework materials and the presence of impurities in flue gas such as water, O_2, NO_x, and SO_x. We review our recent computational efforts in understanding the behavior of MOF materials for gas separations. In particular we will refer to our results using ab initio and density functional theory as well as Grand Canonical Monte Carlo and classical molecular dynamics methods. We will address important practical aspects of MOFs such as the effect of the post-synthesis activation processes, as well as their thermal and chemical stability. In addition, we will introduce a new concept based on shape selectivity for the design of effective MOF materials, and we discuss evaluation of MOF-based membranes using molecular simulation techniques.

Biography

Dr. Balbuena received a Ph.D. in chemical engineering from the University of Texas at Austin. She was Assistant and then Associate Professor at the University of South Carolina, and since 2004, she is Professor of Chemical Engineering, and Materials Science and Engineering at Texas A&M University. Her research focuses on first-principles computational design of materials and processes, with applications to lithium-ion batteries and fuel cells, catalyzed growth of single-walled carbon nanotubes, hydrogen storage, and gas separations using porous materials. She is author of more 180 peer-reviewed articles and co-editor of five books in her fields of specialization.