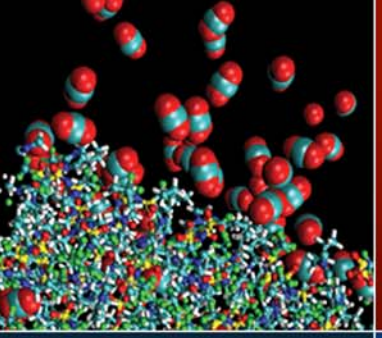

UNIVERSITY OF NOTRE DAME

Department of Chemical and Biomolecular Engineering

SPRING 2015

Graduate Seminar Series

Computational design and development of metal-organic frameworks (MOFs) for energy and environmental applications

Tuesday, April 21, 2015, 3:30 pm

Eck Visitors Center Auditorium

Seminar
3:30 – 4:30 pm

The discovery of advanced materials is essential to the development of novel technologies to address challenges related to the production, storage and efficient use of energy, as well as environmental applications. However, the design, development and commercialization of a new material can take several decades. On these grounds, in 2011, the White House launched a multimillion dollar program, the Materials Genome Initiative (MGI), aiming to accelerate material discovery. In this context, molecular simulation is a powerful tool that can help explore the material space at a significantly faster rate and lower cost than it can typically be done experimentally. This helps focus experimental efforts only on the most promising systems. Here, I illustrate the application of molecular simulations, automated construction algorithms of material molecular models, and computational screening strategies to the design of cutting-edge crystalline materials such as metal-organic frameworks (MOFs).

Metal-organic frameworks are porous materials composed of inorganic nodes and organic linkers assembled into crystalline networks of diverse topologies. MOFs are promising materials for applications such as gas storage, separation and catalysis, because the possibility to vary the combination of building units engenders remarkable tunability of MOF textural and chemical properties. This, however, also means that there are millions of potential MOF structures that could be synthesized, and thus one of the major challenges is to quickly identify the structures that are optimal for a given application. Here, I discuss the use of grand canonical Monte Carlo (GCMC) simulations and other computational methods to evaluate the performance of thousands of hypothetical MOFs generated by different automated construction strategies. The performance assessment centers on energy applications such as methane and hydrogen storage for alternative fuel vehicles, and environmental applications such as pre-combustion carbon dioxide capture. Through computational screening, promising structures were identified which were then synthesized and tested by experimental collaborators. Additionally, structure-property relationships were generated with the goal of providing guidelines for the synthesis of optimal materials and helping to discern material performance limits.

Dr. Diego Gomez-Gualdron holds a doctoral degree in Materials Science and Engineering from Texas A&M University. He is currently a Postdoctoral Fellow in the Department of Chemical and Biological Engineering at Northwestern University. His research interests focus on the use of molecular simulation and computational methods to (help) design and develop advanced crystalline materials.

Dr. Diego Gomez-Gauldron
Northwestern University

For more information visit:

CBE.ND.EDU/SEMINARS