

## LABORATORY SPOTLIGHT CARREON LAB

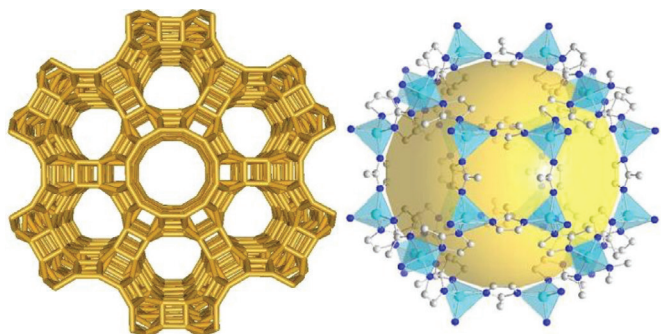


Group members left to right; James Crawford, Moises Carreon PhD, Shurraya Denning, Courtney Smoljan, Jolie Lucero, Taylor Self, Ricardo Ocampo, Carla Osuna

## Welcome to the Carreon Lab!

Here at the Carreon lab in Chemical Engineering, our research is focused on the development and application of functional porous materials on the nanoscale. In essence, porous materials are those made up of a skeletal matrix that frames geometric pockets of fluid, ultimately forming a highly ordered structure. On the very small scale, these materials have many functional applications ranging from binary and higher order gas separations, heterogeneous catalysis, and effective gas storage. Some notable porous materials studied by our student researches include zeolites, porous organic cages (POCs), and metal organic frameworks (MOFs).

\* **Zeolites** are a crystalline material composed of alumina and silica, organized in a three-dimensional tetrahedral structure. Zeolites display micro-sized pores, making them ideal for use in molecular gas separation. The most common application of zeolites in this field is therefore in selective membranes.



**FIGURE 1:** An example nanoscale framework of a porous material

\* **Porous Organic Cages** are covalently bonded structures that assemble into crystalline microporous materials as discrete particles. POCs are an emerging material with promising potential. Notably, they have been employed in gas chromatography separations and in the separation of rare and expensive noble gases such as Xe and Kr.

\* **Metal Organic Frameworks** are crystalline compounds that consist primarily of metal clusters which coordinate to rigid organic structures. A special type of MOF is the zeolite imidazolate framework, or the ZIF. ZIFs use transition metal ions within their clusters and offer a large, accessible pore volume for gas separation and storage.

## Current Members



### Moises Carreon PhD, Principle Investigator

Associate Professor, Colorado School of Mines  
 Chemical and Biological Engineering Department  
 B.S. Chemical Engineering, U.M.S.N.H. Mexico  
 M.S. Materials Science Engineering, U.M.S.N.H. Mexico  
 Ph.D Chemical and Materials Engineering, University of Cincinnati

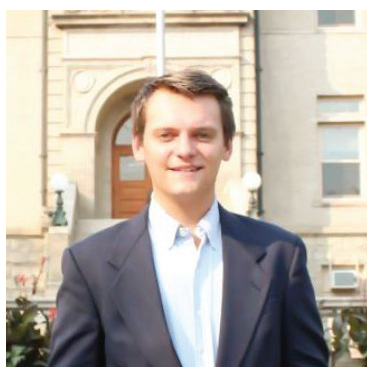
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### Jolie Lucero, PhD Candidate

My research revolves around porous crystals, in particular Porous Organic Cages CC2 and CC3. This material is a subset of functional microporous materials which can be used for a variety of applications such as gas adsorption, gas separations, chiral separations, catalyst supports, sensors, etc. These cage molecules are discreet, purely organic, solution processable, and have uniform micropores which make them attractive for membrane separations. My thesis work is to understand the nucleation and growth mechanisms of these porous crystals, to improve their structural, textural, and morphological properties. Recently, we have published a time-dependent growth study of CC3, in which we have concluded that experimental synthesis time (in conjunction with simulation studies), effects final material properties such as gas adsorption, Brunauer-Emmet-Teller (BET) surface areas, crystal morphology, and crystal lattice expansion/contraction.



J. Lucero, S.K. Elsaidi, R. Anderson, T. Wu, D. A. Gómez-Gualdrón, P. K. Thallapally, M. A. Carreon. *Cryst. Growth Des.* 2018, 18, 921–927.



### James Crawford, PhD Candidate

I am interested in understanding catalysis at the molecular level. By tailoring green chemistry approaches, we are able to tune both the architecture and the chemistry of our systems at the sub-nanometer scale. We are applying these catalysts to the deoxygenation of bioderived products in pursuit of renewable and scalable biofuels. In our most recent work, we have been focusing on the use of low cost, earth abundant, and highly active transition metals including nickel and cobalt for the production of biodiesel [1]. Continued research on non-noble metal catalysts could change the technoeconomic outlook for fatty acid derived biofuel by replacing the cost prohibitive platinum or palladium [2]. In future work I am interest in pursuing in-situ analysis of both chemical reactions and catalyst characterization.

[1] Crawford, JM; Carreon, MA. Decarboxylation of Diunsaturated Linoleic Acid to Heptadecane over Zeolite Supported Pt/ZIF-67 Catalysts. *Ind. Eng. Chem. Res.* 2018, 57 (47), 15991–15997

[2] Crawford, JM; Smoljan, CS; Lucero, J; Carreon, MA. Deoxygenation of Stearic Acid over Cobalt-Based NaX Zeolite Catalysts. *Catalysts* 2019, 9(1), 42.



## Shurraya Denning, PhD Candidate

The research I am conducting involves determining if gas hydrates can act as a membrane to remove impurities from natural gas, such as carbon dioxide, nitrogen, and hydrogen sulfide. Gas hydrates consist of water molecules that form a hydrogen bonded crystalline structure around a guest gas molecule, typically under the conditions of high pressure and low temperature. If harnessed properly, a gas hydrate may form around one type of gas molecule and not another. Preliminary simulations from the Colorado School of Mines Gibbs Energy Minimization algorithm (CSMGem) indicate that by fine tuning the temperature and pressure conditions, gas hydrates can selectively form using the impurities found in natural gas rather than the desired product, methane. This separation process is advantageous due to its environmentally benign nature as it only requires water, high pressure, and low temperatures to form the hydrates. My thesis work consists of investigating the hydrate phase equilibria for common raw natural gas compositions, designing a gas hydrate membrane process, characterizing and determining the kinetics of the gas hydrates, and optimizing the separation performance of the gas hydrate membrane.

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## Carla Osuna, Undergraduate Researcher

My research in Dr. Carreon's lab has been dedicated to better understanding the characteristics of Porous Organic Cages. POCs are microporous crystals with high surface areas and uniform micropores. POCs have applications in many chemical processes including gas separations, catalysis driven reactions, and even water desalination, as recent studies have found [1]. I have examined the effects in morphology and particle size of CC3 when pyrolyzed in an inert gas environment. Additionally, I have been synthesizing CC2 and experimenting with various synthesis conditions in order to produce a crystalline material of high quality and yield with consistency.



[1] Kong, Xian, and Jianwen Jiang. "Porous Organic Cage Membranes for Water Desalination: a Simulation Exploration." *Physical Chemistry Chemical Physics*, Royal Society of Chemistry, 28 July 2017.



## Ricardo Ocampo, Undergraduate Researcher

My research focuses on zeolite imidazole frameworks, or ZIFs, which are a subclass of metal organic frameworks, or MOFs, that have drawn significant research interest in recent years. Due to higher levels of CO<sub>2</sub> emissions and an increased demand for natural gas as a global fuel source, which requires CO<sub>2</sub> extraction, the need to develop new ways of removing CO<sub>2</sub> has significantly increased. Membranes are an excellent alternative to conventional methods of removing CO<sub>2</sub>. Membrane-based gas separations offer an energy-efficient, economical, and environmentally friendly alternative to traditional separation methods (e.g., cryogenic distillation). ZIF-12, in particular, has proven to be successful in separating CO<sub>2</sub> and CH<sub>4</sub> [1]. As part of my research, I have been creating ZIF-12 membranes through various methods (e.g. solvothermally, room temperature, microwave, etc.) and characterizing it using: XRD, BET, TGA, and SEM.

[1] G. Yilmaz, A. Ozcan, and S. Keskin, "Computational screening of ZIFs for CO<sub>2</sub> separations," *Molecular Simulation*, vol. 41, no. 9, pp. 713–726, 2014.



## Taylor Self, Undergraduate Researcher

In the lab, my work also primarily deals with ZIFs. I have studied many different kinds of ZIF, including ZIF-8, ZIF-67, and ZIF-11. The primary differences between these materials is the metal ions which serve as a key component of their structure. In ZIF-8 and ZIF-11, the metal clusters are comprised of zinc ions, whereas in ZIF-67, they are comprised of cobalt. I have explored the effects of adding crystal growth inhibitors to my ZIF recipes in considerable detail. The idea here is to add some type of polar solvent, such as olyemine or P123 surfactant, which will create micelles in solution. These micelles incapsulate ZIF crystals, and thus standardize their size and morphology. Uniform crystal size lends itself to increased crystal intergrowth and ultimately more continuous membranes. In past years I have also worked with a type of zeolite called SAPO-34, again with very promising applications as a membrane for binary gas separations. Currently, I have turned my focus back to ZIF-11, and will be exploring the effects of microwave synthesis versus the traditional solvo-thermal process on crystal morphology and functional properties [1].

[1] T. Wu, J. Lucero, J.M. Crawford, M.A. Sinnwell, P.K. Thallapally, M.A. Carreon, *Journal of Membrane Science* 2019, 573, 288-292

J. Sánchez-Laínez, B. Zornoza, Á. Mayoral, Á. Berenguer-Murcia, D. Cazorla-Amorós, C. Téllez, J. Coronas, “Beyond H<sub>2</sub>/CO<sub>2</sub> Upper Bound: One-step Crystallization and Separation of Nano-sized ZIF-11 by Centrifugation and its Applications in Mixed Matrix Membranes,” *Journal of Materials Chemistry A*, vol. 3, no. 12, pp. 6549-6556, 2015.

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## Courtney Smoljan, Undergraduate Researcher

My research involves the synthesis and characterization of new non-noble metal, porous media catalysts and the conversion of biomass to hydrocarbon chains over these catalysts. The purpose of the project is to find an economical renewable fuel produced over an inexpensive catalyst that can help reduce CO<sub>2</sub> emissions and leverage new bio-resources. Recently, we have documented an example of these novel non-noble metal catalysts [1]. I am currently exploring the synthesis of mesoporous catalysts.



[1] Crawford, JM; Carreon, MA. Decarboxylation of Diunsaturated Linoleic Acid to Heptadecane over Zeolite Supported Pt/ZIF-67 Catalysts. *Ind. Eng. Chem. Res.* 2018, 57 (47), 15991–15997

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- X. Feng, Z. Zong, S.K. Elsaidi, J. B. Jasinski, R. Krishna, P. K Thallapally, M.A. Carreon, *Journal of the American Chemical Society* 2016, 138 (31), 9791-9794.
- S.R Venna, M.A. Carreon, *Journal of the American Chemical Society* 2010, 132 (1), 76-78.
- S.R Venna, J.B. Jasinski, M.A. Carreon, *Journal of the American Chemical Society* 2010, 132 (51), 18030-18033.
- C.M. Miralda, E.E. Macias, M. Zhu, P. Ratnasamy, M.A. Carreon *ACS Catalysis* 2011, 2 (1), 180-183.