Computer-accelerated discovery of advanced porous crystals: Are we there yet?

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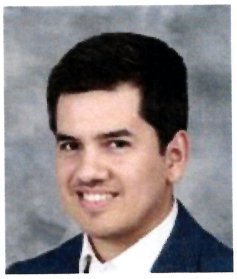
Abstract: Many of the most important scientific challenges of the 21st century require the discovery of new materials with unprecedented properties. Due to the possibility of exquisite chemical and structural control at the nanoscale, in many areas, scientists have been waiting for porous crystals such as metal-organic frameworks (MOFs) to provide the required properties. However, discovering breakthrough-enabling MOFs for a given application is akin to "finding a needle in a haystack" due to the overwhelmingly number of different MOFs that could be synthesized. Accordingly, high throughput computational screening of MOFs emerged seven years ago with the promise of using molecular simulations to quickly discover the best materials for each application of choice from large MOF databases. *But to what extent has this approach been successful?*

In this talk, I will discuss past and current efforts on using molecular simulation to accelerate the understanding and discovery of MOFs for molecular storage and delivery, chemical separations and catalysis. I will present some success stories that led to the synthesis of new materials, while also discussing the challenges that need to be overcome to truly make computational discovery effective, and efforts in my lab to overcome those challenges. These efforts include multiscale integration of quantum mechanics, classical mechanics and machine learning, as well as computational synthesis and crystal prediction methods.



Dr. Diego Gómez-Gualdrón is an Assistant Professor in the Department of Chemical and Biological Engineering at Colorado School of Mines. Dr. Gómez-Gualdrón holds a bachelor's degree in Chemical Engineering from Universidad Industrial de Santander in Colombia, and a doctoral degree in Materials Science and Engineering from Texas A&M University. Before joining Mines, he was a Postdoctoral Fellow in the Department of Chemical and Biological Engineering at Northwestern University. Dr. Gomez-Gualdron's research interests focus on the use of molecular simulation and computational methods to discover advanced materials. He has authored or co-authored over 40 publications. He is the recipient of a Silver Graduate Student Award from the Materials Research Society (2012), and an Outstanding Researcher Award from the International Institute of Nanotechnology at Northwestern University (2014), and the NSF CAREER Award (2019).

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