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The interview with the author of the PhD thesis:
„Computational crystal structure and property prediction of metal-organic frameworks"

Could you tell our readers about your journey into this field of research?

My journey into this field of research has been driven by a deep curiosity about the materials that make up our world and how we can engineer them for impactful applications. During my academic path, I was especially drawn to computational chemistry because of its ability to model and predict different material properties with remarkable precision and efficiency. This interest led me to focus on metal-organic frameworks (MOFs), which are incredibly versatile materials with tunable properties. What excited me most was their potential in a diverse range of areas like gas storage, separation, and even energetic materials – applications that have real-world impact for clean energy, environmental sustainability, and safety. The fundamental motivation for my research is to apply theoretical insights to pursue practical solutions that can address some of today's most pressing challenges.

Could you explain in simple terms what metal-organic frameworks are and why predicting their structures is particularly challenging?

Metal-organic frameworks (MOFs) are a class of highly versatile material which consists of metal centres or clusters joined by organic molecule linkers to form 3D porous polymeric structures. There are already so many exciting applications of MOFs from a diverse range of industries that are beneficial for our society, such as fuel transportation, greenhouse gases absorption, water purification, platforms for drug delivery, catalysts, hypergolic fuels and many more.
Since the key principle behind all various application of MOFs is directly related to the chosen metal node and linker composition, in principle, there are unlimited combinations one can try for desired properties. Moreover, compared to molecular crystals or inorganic materials, MOFs are polymeric, meaning that the whole repeating framework is a single molecule without any inter- or intramolecular separations. Such a phenomenon has made predicting MOF structures more challenging as well as computationally demanding than aforementioned structures. From my research along with my co-workers, we have addressed this prediction challenge using the *ab initio* random structure search (AIRSS) method along with Wyckoff Alignment of Molecules (WAM) algorithm which utilise symmetry to dramatically increase the overall computational efficiency to obtain accurate MOF structures with desired properties in a systematic manner.

What was the most interesting discovery you made during your research?

The most interesting discovery of my research was the prediction of a series of previously unseen hypergolic MOFs, for the potential replacement of highly toxic and carcinogenic hydrazine-based rocket fuels. This breakthrough was achieved through our *ab initio* crystal structure prediction (CSP) method for MOFs supported by experimental validations, marking a significant advancement in the design of safer and more sustainable propellants.
In the study, we utilized CSP to explore the structural landscape of MOFs composed of energetic ligands and hypergolic linkers. By systematically varying organic linkers, we identified novel MOF structures exhibiting spontaneous ignition upon contact with oxidizers – a hallmark of hypergolic behavior. These computational predictions were subsequently confirmed through experimental synthesis and testing, demonstrating the efficacy of CSP in guiding the discovery of functional materials. The implications of this work extend beyond aerospace propulsion, highlighting a pathway toward the design of advanced materials for a variety of technological applications.

In what ways can your research findings be translated into practical applications or real-world solutions?

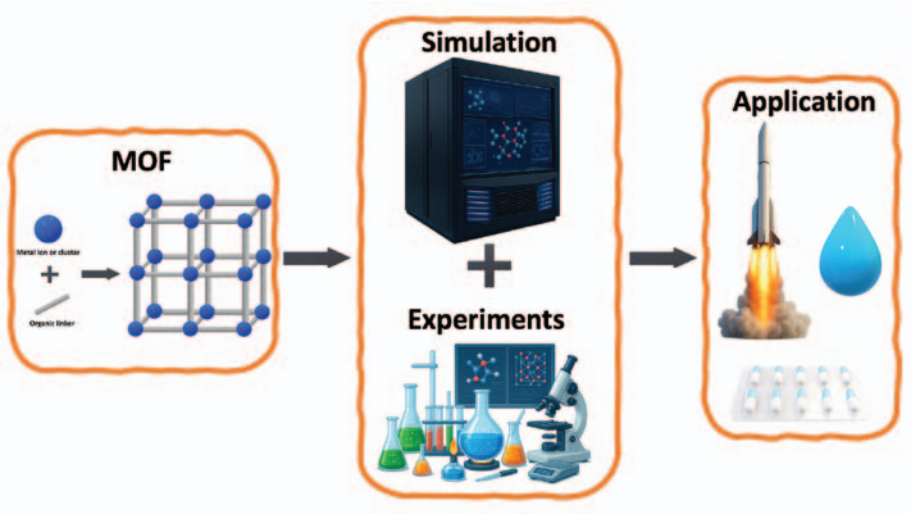
The major driving force for my research is to improve the efficiency of designing MOFs with tailored applications. By developing computational tools and predictive models, my work aims to streamline the discovery of MOFs with specific properties – whether it's for gas storage, separation, catalysis, energetic materials and many more. These findings can be directly translated into practical applications by reducing the time and cost associated with experimental trial-and-error. So far, such idea of designing MOFs has already been showcased from one of my latest published works (DOI: 10.1021/jacs.2c12095) where novel non-toxic MOF-based propellants have been found. Overall, my research can support a more targeted and efficient path from molecular theory to functional MOF design.

What was the contribution of the Cyfronet supercomputing infrastructure to your research?

Cyfronet's supercomputing infrastructure played a critical role in my research for executing all necessary calculations for the design of MOFs computationally with desired properties. Specifically, I used CPU core clusters on both the Prometheus and Ares supercomputers to perform the majority of crystal structure prediction (CSP) calculations for MOFs, which are computationally intensive and require exploring vast configurational spaces with high accuracy. These resources enabled me to run thousands of periodic density functional theory (DFT) simulations in parallel, significantly accelerating the structure generation and screening processes. Moreover, the GPU cores offered by the Ares supercomputer were essential for training machine learning potentials, in order to further speed up the CSP calculations for MOF design. These models require handling large datasets and optimizing complex neural network architectures, which would be infeasible on standard hardware. By leveraging GPU acceleration, I was able to efficiently train models that can predict MOF structure and properties with near DFT-level accuracy, but at a fraction of the computational cost.

What advice would you give to those considering a career in science?

My biggest piece of advice is to follow your passion and let your curiosity lead the way. A career in science goes beyond memorizing facts or solving equations – it's about asking and solving the questions that matter to you. If there's a topic that fascinates you or a problem you can't stop thinking about, that's a strong indication you're on the right path. More importantly, please remember it's okay not to have everything figured out from the start and focus on solving one question at a time. Finally, keep in mind that science is not just a solo game, and don't be afraid to reach out the others for help.



Schematic overview of the design workflow for tailored metal-organic frameworks (MOFs): computational simulations via crystal structure prediction (CSP) method, guiding the discovery of promising MOF candidates, followed by experimental validation to realize targeted applications.