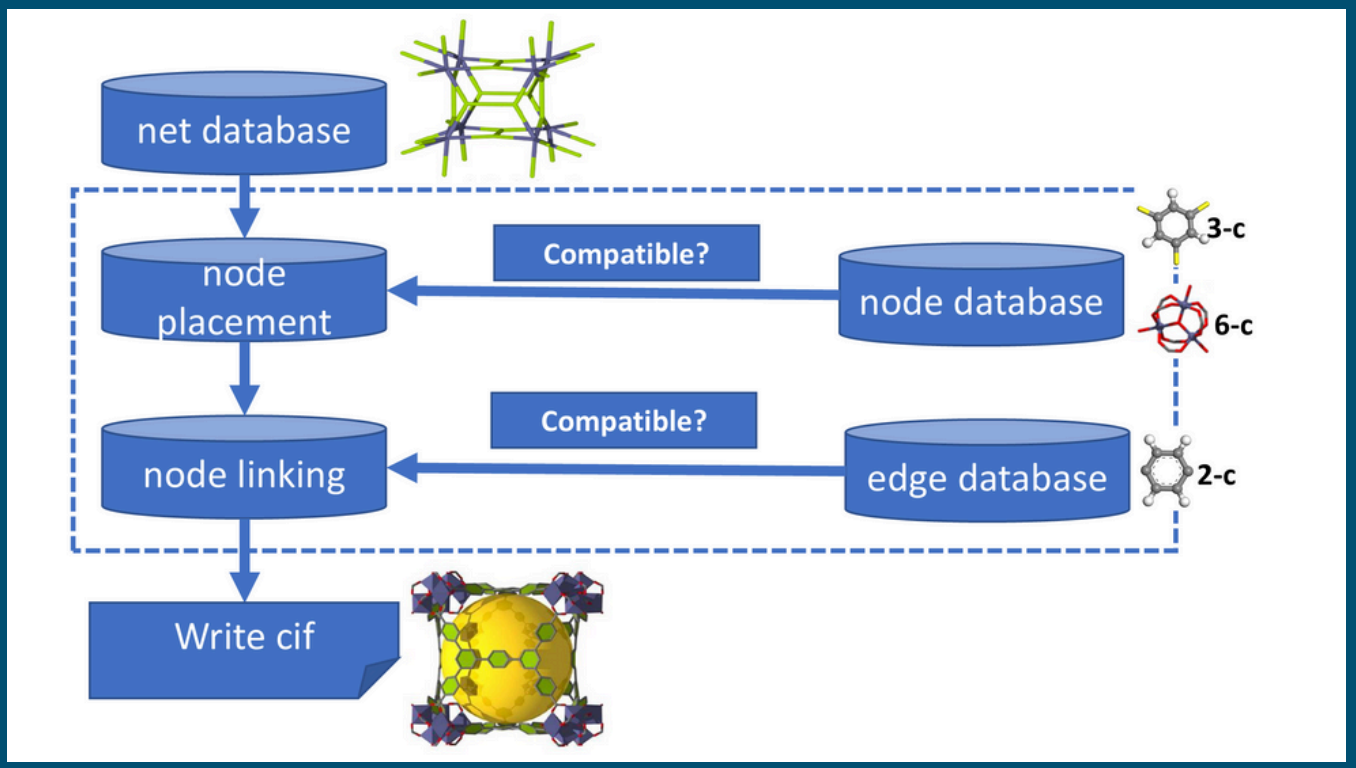
MOST-H_2



MOF DATABASE AND SYNTHESIZABILITY TOOL

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What inspired the creation of the new MOF database and the synthesizability tool?

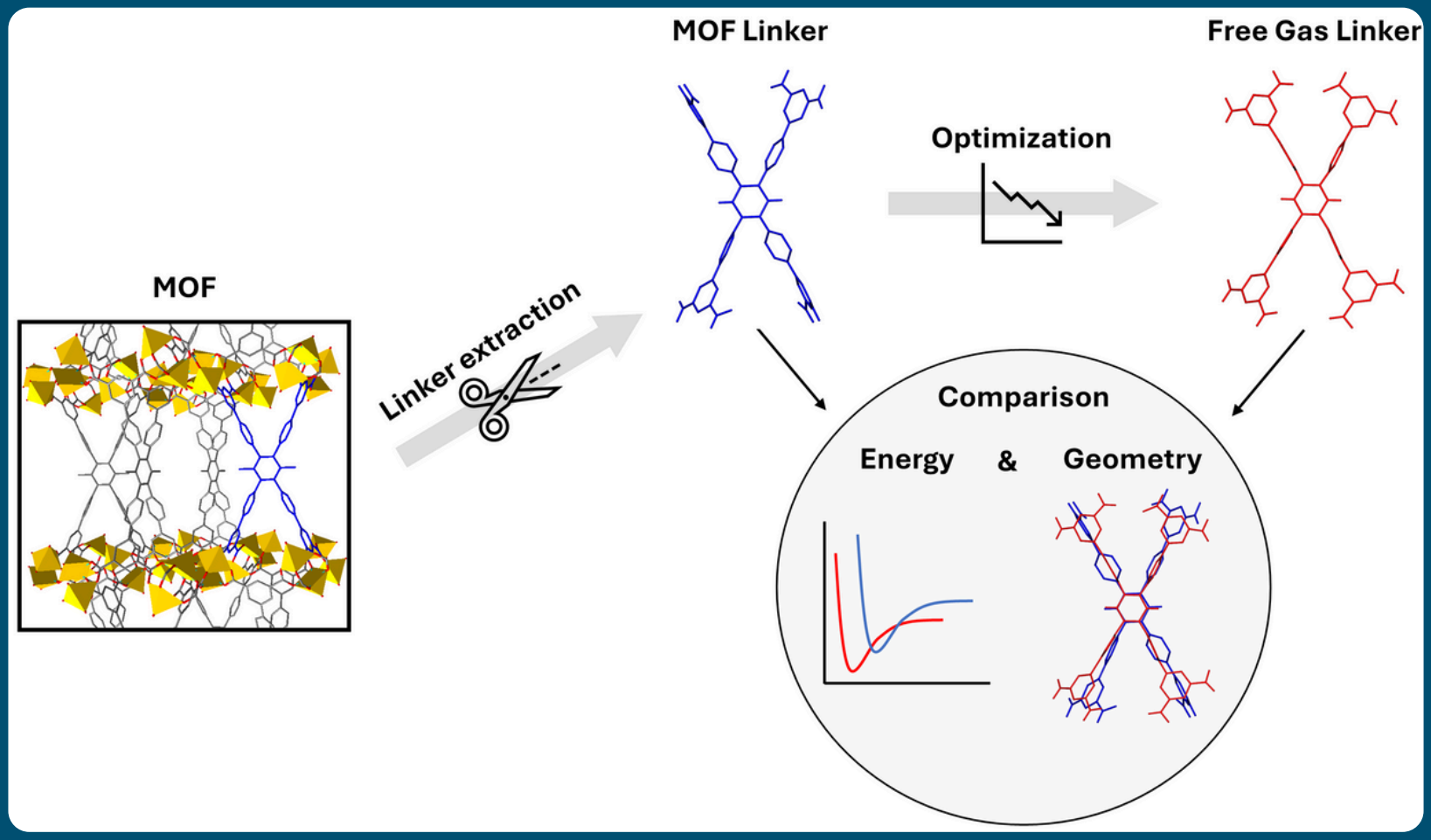
Thousands of MOFs (Metal-Organic Frameworks) have been predicted computationally, but only a fraction have been synthesized. This gap inspired us to create a tool that evaluates synthesizability based on structural stability and linker conformation, bridging theory and practice. The robust and efficient tool is user-friendly, requiring minimal expertise, and helps researchers prioritize MOFs with the best potential for real-world applications.

Which databases of MOFs did you analyse, and what insights did you gain?

We analyzed QMOF, CoRE MOF, and ToBaCCo, covering over 40,000 MOFs. QMOF and CoRE MOF contained the most promising candidates due to optimized, stable materials, while ToBaCCo showed lower synthesizability due to non-optimized structures. These findings guide researchers toward instances with higher chances of synthesizability.

How does the tool assess whether a MOF is synthesizable?

The tool evaluates energy and geometrical differences by comparing the linker's behaviour in the MOF structures to its free-gas state. MOFs with minimal strain and energy disparities are more stable and feasible to synthesize. This process helps identify MOFs with real-world synthesis potential, moving beyond theoretical predictions.



How does this study contribute to the MOST-H2 project goals?

The tool and database support MOST-H2 by identifying MOFs that are stable, synthesizable, and optimized for hydrogen (H2) storage. By focusing on materials with high hydrogen storage potential, the study accelerates the discovery of efficient and cost-effective solutions for sustainable energy systems.

What are some of the broader benefits of the synthesizability tool?

The tool enables efficient MOF screening for applications like gas storage, catalysis, and drug delivery. It also generates data for machine learning, paving the way for AI models to predict synthesizability more accurately. With AI, researchers can explore underutilized areas of MOF design and discover materials with exceptional properties.

How do you see the tool and database evolving in the future?

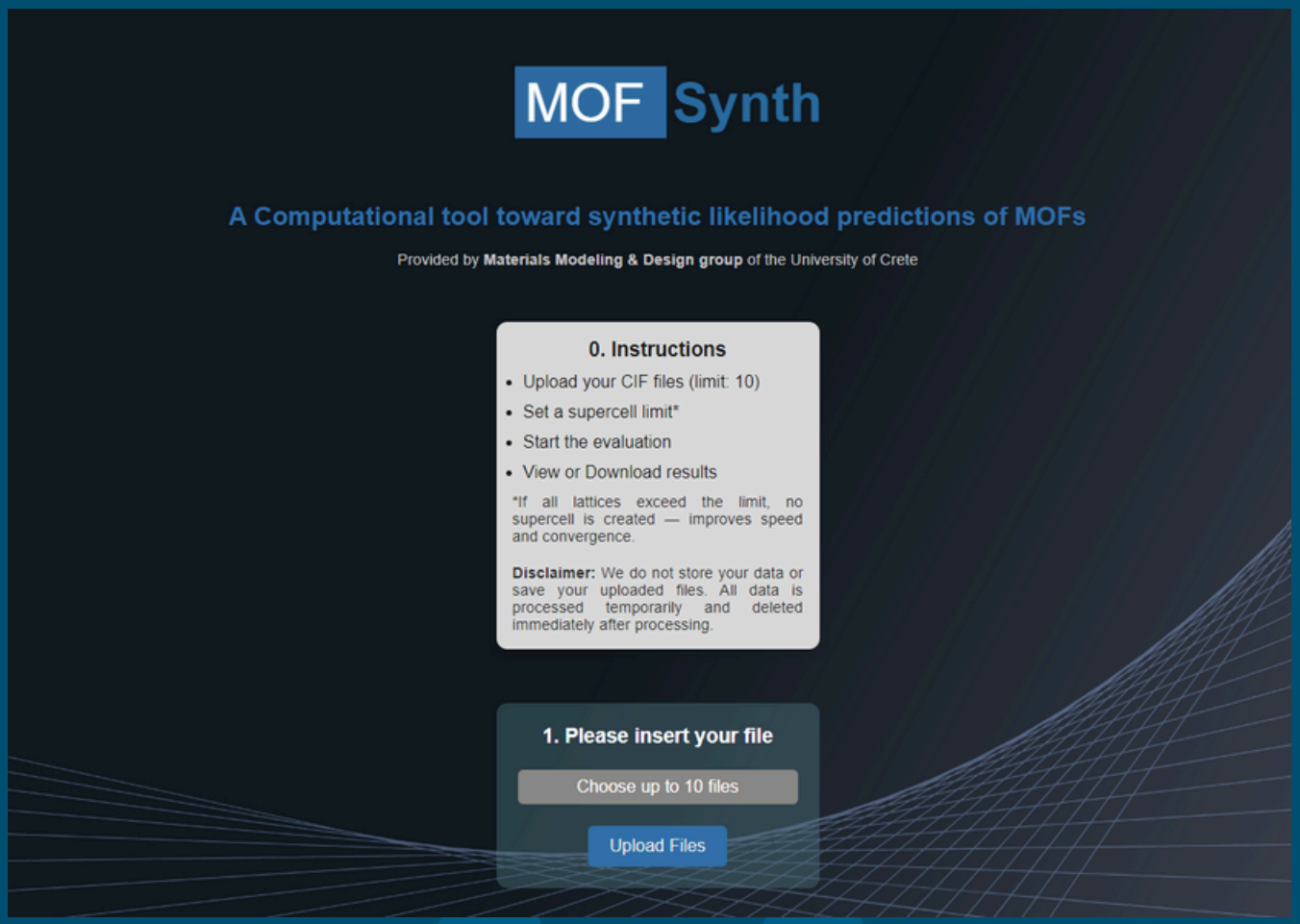
Future plans include integrating machine learning for higher precision in synthesizability predictions and expanding the tool to other materials like COFs (Covalent Organic Frameworks) and ZIFs (Zeolitic Imidazolate Frameworks). This evolution will broaden its impact, supporting interdisciplinary research and driving discoveries across a wide range of advanced materials.

Thank You

Try it for yourself!

The MOFSynth web application allows researchers even with minimal computational knowledge to use the evaluation tool and extract information on MOFs of their choice.

https://mofsynth.website



Learn more about UoC

UNIVERSITY OF CRETE

The University of Crete is a recognized research and academia institution. The department of chemistry combines long standing expertise and great achievements in the design and synthesis of novel MOFs and the development of advanced computational methodologies incl. machine learning techniques for MOF large-scale screening. The University of Crete has been awarded with the “HR Excellence in Research Award”.