

Synthesizability: The Open Question in Digital MOF Discovery

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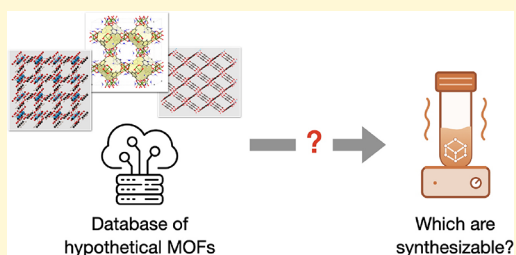


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ABSTRACT: The growing number of hypothetical metal–organic frameworks (MOFs) has created a need for reliable methods to identify candidates that can be synthesized experimentally. This Viewpoint examines current computational approaches to the evaluation of MOF synthesizability, grouping them into thermodynamic, strain- and mechanics-based, and data-driven methods. Thermodynamic studies evaluate formation enthalpies or free energies, stability relative to competing phases, and can include solvent effects. Structural approaches quantify linker deformation and mechanical stability as a proxy for viability of a hypothetical structure. Data-driven machine learning models use geometric, topological, or chemical relationships to known materials as a way to estimate synthesizability. We review the recent advances of these approaches, their strengths and their limitations, noting that at the present time, there is no silver bullet to solve this open challenge. Future progress will require combining complementary methods and using consistent experimental data to refine computational models and allow the identification of candidates for synthesis in screening studies.



The discovery of novel metal–organic framework (MOF) structures is a fast-paced area of research with a vibrant community. In this area, as in many other research fields, data-driven methods offer the prospect of moving beyond the standard methods of materials discovery, based on trial-and-error, chemical intuition, systematic exploration of synthetic space, and serendipity. Computational methods based on the principles of reticular and coordination chemistry have been used for more than 15 years to create databases of hypothetical MOF structures, by combinatorial assembly of predefined building blocks¹ or topology-based crystal construction.^{2–4} More recently, advances in generative artificial intelligence (GenAI) in the field of materials science have been rapid: generative models to create novel crystalline structures are commonly applied to inorganic materials,⁵ and are now being used to propose new MOF structures within the constraints of their specific chemistry.⁶ Such methods of enumeration or exploration of the MOF chemical and structural space are typically coupled with high-throughput computational screening workflows for specific applications, to select top-performing candidate materials for selected physical and chemical performance indicators.⁷

The principles of reticular and coordination chemistry combine to make the number of possible MOF structures infinite, and several databases of hypothetical MOFs contain millions of materials in total. Yet, only about 100,000 MOFs have actually been reported to date;⁸ this discrepancy is the core of the question of synthesizability (or, put differently, of experimental feasibility), which remains one of the great open challenges in our field of research: given a hypothetical structure, how likely is it that it can be synthesized?^{9,10} The question has several

ramifications, including the identification of specific synthetic procedures, or the imposition of constraints on the resources that can be allocated for the synthesis: can a material be obtained in a given time, with a limited number of starting materials, within a fixed budget, or with a green chemistry pathway? This is one of the hardest, and therefore least often addressed, questions of the AI-assisted discovery of MOF materials. However, it has a fundamental relevance for the discovery of novel materials in the real world, limiting the number of hypothetical structures that can actually be made in the lab (and therefore, later, translated to applications).

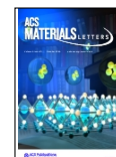
But while the problem remains unsolved, there have been several recent efforts to address this elephant in the room in the digital discovery pipeline for MOFs. We will present these recent attempts at quantifying the feasibility and stability of MOF structures, through several different proxies, such as thermal, mechanical and chemical stability, as well as experimental synthesizability. We will also contrast the situation of MOFs with related families of compounds, where the field is more advanced, such as in zeolites and dense inorganic compounds — suggesting some possible inspiration for future research.

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The first family of approaches to the question of experimental feasibility has been to link synthesizability to the thermodynamic stability of the MOF framework. This approach draws on earlier findings that, while MOFs like other nanoporous framework materials can display an important degree of polymorphism, there are strong links between the thermodynamic stability of the framework, its density, and its experimental likelihood of synthesis.^{11,12} Building upon that background, in 2020, Anderson and Gómez-Gualdrón¹³ proposed the first large-scale study of the synthetic likelihood of MOFs through the calculation of free energies. In order to achieve this high-throughput scale, they had to use a computational method with relatively low computational cost, and therefore significant approximations, such as the use of simple “universal” force fields and some ad hoc corrections to account for the metal/linker ratio. In doing so, they could identify that all experimentally synthesized MOFs within their data set clustered below a free energy threshold of a few kJ/mol. This highlighted that a low free energy is a necessary, but not sufficient, condition for a MOF to be synthetically accessible. It is exemplified in Figure 1 (left panel), where the threshold is visible as an orange line; it is also clear from the graph that not all the MOFs below the free energy threshold have been experimentally synthesized.

From the seminal work of Anderson and Gómez-Gualdrón,¹³ the necessity to go deeper is highlighted by two facts. First, not all MOFs with low free energy are experimentally realized. Second, there are cases in which, in a family of MOF polymorphs, the synthesized one is not the lowest free energy structure (about 20% of such occurrences). Several recent works have therefore tried to improve various aspects of the use of thermodynamic metrics as a proxy for experimental synthesizability. Wu et al.¹⁵ have proposed an acceleration of the free energy calculation, developing a deep-learning predictor that speeds up the evaluation of synthetic likelihood and can scale to tens of thousands of hypothetical MOF structures. Their predictor is based on the transformer-based TabPFN framework,¹⁶ and trained against classical molecular dynamics results. A similar deep-learning approach was also taken by Niyongabo Rubungo et al.¹⁷ these authors introduced a sequence representation of MOFs, incorporating both local and global MOF features, as input to a large language model for free energy prediction.

In a different approach, Dallmann et al. recently performed a large-scale density functional theory (DFT) study of more than 20,000 MOFs and coordination polymers, in order to compute their formation energies.¹⁸ This strategy is complementary to the free energy methods presented above: it has the advantage of allowing a more accurate computation of the energy (at the quantum chemical level, rather than relying on “universal” classical force fields). On the minus side, it neglects the entropic aspects of the stability, which can be an important contribution for MOFs due to their high number of degrees of freedom.¹⁹ On the basis of these energy calculations, Dallmann et al. constructed convex hull phase diagrams²⁰ and argued for the use of the energy above hull as a synthesizability metric for hypothetical MOFs — one that has proven very powerful in other families of materials, and in particular in dense inorganic crystals.^{21,22}

However, MOFs are different from dense phases because of their porosity. Most MOFs are thermodynamically metastable,²³ i.e., they lie above the global energy minimum — but not by too much. They have a thermodynamic penalty associated with their porosity, and their experimental existence therefore depends on kinetic trapping, and is linked to the conditions

of their synthesis. Moreover, solvent and other molecules are present in the nanopores during synthesis, and their influence can have a major impact as the favored phase will often not correspond to the most stable evacuated framework. Fajardo-Rojas et al. proposed a methodology to account (at least in part) for this influence of the synthesis environment that is absent from previous dry-crystal stability metrics. This work parallels, in a way, the computational work performed to better understand how the presence of template molecules (or structure-directing agents) affects the energetic ordering of zeolite topologies and the synthesis of specific structures.^{24,25} Fajardo-Rojas et al. performed calculations of heats of adsorption and solvation free energies in MOFs for four common solvents (DMF, water, methanol, and *n*-hexane).²⁶ Because calculations of solvation free energies are computationally expensive, they introduced an extrapolation protocol based on partially solvated structures. Their findings highlight that solvent stabilization can reverse the intrinsic stability order of MOFs among a family of polymorphs. Although that work has not yet been scaled up to a more systematic level, it is a promising step in the direction of including solvent effects in the evaluation of MOF synthesizability — and future work may also consider the influence of temperature.

Although thermodynamic stability is a good proxy for synthesizability in dense materials, we have seen that nanoporous frameworks, by their very nature, are designed to be metastable phases. Therefore, approaches that avoid relying on formation energy (or free energy) have been proposed as alternative views of MOF stability.

Livas et al. proposed in 2024 the MOFSynth methodology, whose goal is to estimate the synthetic likelihood of MOFs based on the strain of the framework structure.¹⁴ They decompose each material into its constituent building blocks, focusing on the organic linkers, and comparing the energy and geometry between the linker conformation within the MOF structure and its isolated, relaxed state (see Figure 1, right panel). This approach is local (not global) and therefore has relatively cheap computational cost, making it suitable for large-scale screening of databases. Moreover, it is based on chemical intuition and can be easily interpreted: a high deformation energy or large geometrical change indicates an implausibly strained linker.

In their original 2024 paper,¹⁴ Livas et al. applied their methodology to more than 40,000 MOFs from existing databases, with energy evaluation performed at the classical level with a UFF force field. In later work, the same group extended their implementation to a new version of the tool, named MOFSynth-ADV, with greater capabilities.²⁷ In particular, they demonstrated the possibility of using more accurate energy calculations for the linkers, through either extended tight-binding (xTB)²⁸ or machine learning interatomic potentials (MLIP).²⁹

One can generalize this concept of structural strain as a proxy for feasibility by considering, more broadly, the mechanical stability of the hypothetical MOF structures as a criterion for high-throughput screening. This is an idea that has proven useful in the field of zeolites, where a previous study showed that in order to be experimentally feasible, hypothetical zeolite structures need not only to have low formation energy, but they also require some degree of mechanical stability.³⁰ When it comes to MOFs, it has been clearly demonstrated that there is a balance to achieve between porosity and mechanical stability,³¹ and that MOFs can display a wide range of mechanical properties, heavily influenced by chemical composition, geometry and

Evaluation of MOF synthesizability based on:

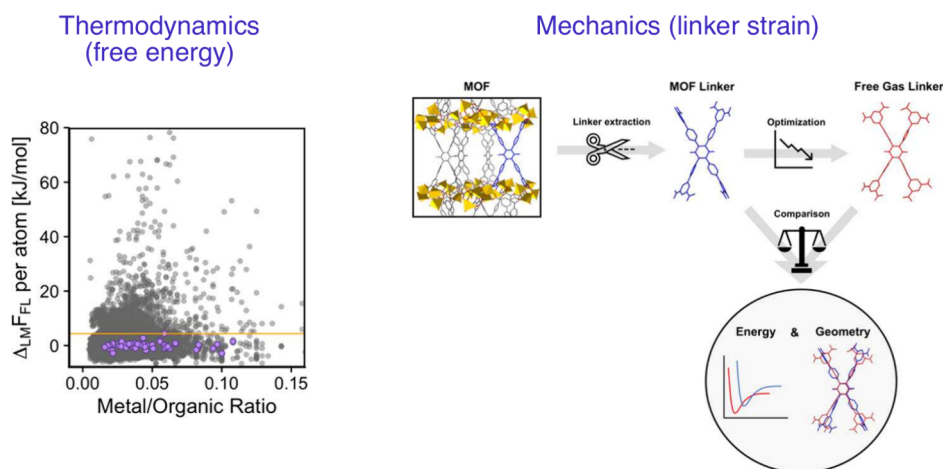


Figure 1. Two methods for the evaluation of MOF synthesizability. Left: Distribution of relative free energy ($\Delta_{ML}F_{FL}$) versus metal-to-linker atoms ratio of each MOF. The purple points correspond to 54 previously synthesized MOFs, and the gray points are the remaining 8500 hypothetical MOFs. The horizontal line correspond to a free energy threshold identified as a criterion for synthesizability of a MOF. Reprinted from ref 13. Right: Schematic representation of the MOFSynth workflow: linker extraction, optimization of the isolated linker, comparison of the original and optimized structures and energies. Reprinted from ref 14 under the terms of the CC-BY 4.0 license.

topology.³² Therefore, researchers have worked to incorporate such a criterion in computational workflows, as the field rapidly progressed in evaluating the mechanical stability of frameworks through theoretical methods, at various levels of theory.³³

One such example is the screening study of MOFs for CO₂ capture by Mohamed et al.,³⁴ which incorporated mechanical stability among other factors in their procedure. The authors estimated this from elastic constants obtained through molecular dynamics simulations, and therefore calculated at the same time as thermodynamic stability in the form of free energy. This evaluation was performed at the end of the screening funnel, because it is expensive and can only be performed at the scale of hundreds of materials — although the use of machine learning predictors could reduce in the future the computational cost of mechanical characterization, as promising studies have shown for MOFs³⁵ and other framework materials.³⁶

A third family of approaches to the question of experimental feasibility is to avoid reliance on physics-based proxies and instead use data-driven methods, built on the experimental knowledge available from the published literature. In this philosophy, a hypothetical framework is promising if its local geometry or global topology resembles experimentally realized frameworks, where the crux lies in the definition of “resemblance”. This is a powerful method, because it learns not from computational proxies but from actual experimental data. Moreover, the definition of similarity of structures can be very flexible and can include very rich high-dimensional descriptors. One limitation of this approach is that the “feasibility” that is learned by the models does encode several biases, and has the potential to penalize genuinely novel but accessible structures. Another is that it offers limited interpretability and explainability.

A recent example of this approach is the publication by Lee et al. of a data-driven search algorithm to identify synthesizable zeolitic imidazolate frameworks (ZIFs).³⁷ Within a well-defined chemical space, the authors applied explicit geometrical and topological rules on the tetrahedral networks based on experimentally known ZIF structures to reduce a database of

4.45 million potential zeolitic structures to 420 candidate ZIF topologies. Atomistic models of the corresponding ZIFs were constructed with the topology-based ToBaCCo software,³ optimized with an ab initio-derived ZIF force field to relax their structure, and ranked based on energy. The power of this approach was confirmed by experimental synthesis of three new ZIFs corresponding to two previously unreported topologies: UZIF-31, UZIF-32, and UZIF-33.

The use of less explicit criteria is also possible, relying on higher-dimensional descriptors of the structures and suitable metrics in descriptor-space. While they have not been applied (to our knowledge) to MOFs yet, such a methodology has been used by Helfrecht et al.³⁸ to rank the synthesizability of hypothetical zeolites — a problem very similar to that of MOFs. These authors trained linear support-vector classifiers to distinguish experimental zeolite topologies (only 230 of them are known) from hypothetical structures from the database of Deem and Pophale (more than 300,000 frameworks),³⁹ using Smooth Overlap of Atomic Positions (SOAP) descriptors⁴⁰ to represent the structures. The classifier achieved an accuracy of 95% in distinguishing experimental and hypothetical structures. This approach is very promising and could be extended to other families of nanoporous materials such as MOFs, given that there are a large number of data sets available for both hypothetical and experimental structures.⁴¹

In a related direction, Zhang et al. proposed to evaluate the synthesizability of hypothetical MOFs through data-driven methods, but operating in chemical space rather than topological or geometrical space.⁴² Their approach directly addresses the lack of trustworthy negative synthesis data (i.e., systematic records of failed synthesis attempts) by training one-class classifiers only on experimentally observed metal–linker combinations. This is an interesting direction, although such models are quite difficult to evaluate and validate, and direct confirmation by experimental synthesis has not yet been performed.

Finally, to complete this overview of methods summarized in Figure 2, it is important to note that data-driven approaches have been used in the past few years to go beyond the question

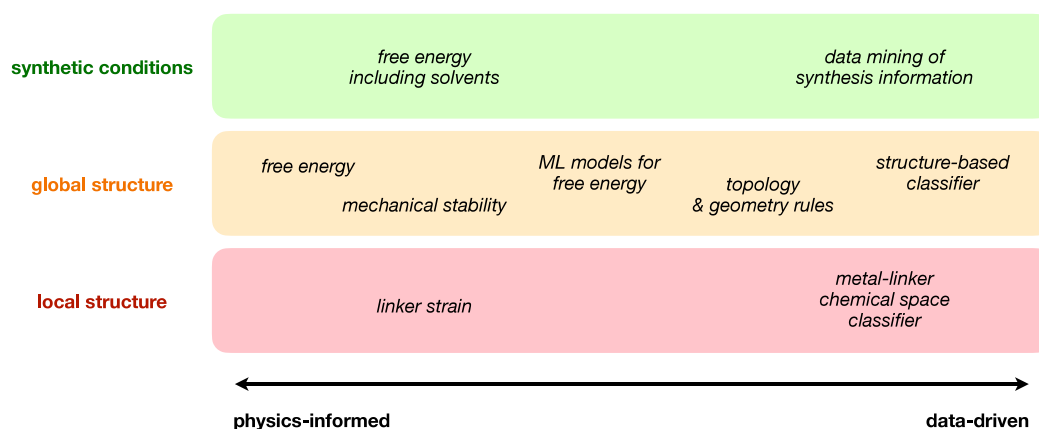


Figure 2. Summary of the different computational approaches to the determination of MOF synthesizability, sorted according to the scale of information used and the nature of the computational workflow.

of whether a material is synthesizable, and actually attempt to predict the synthetic conditions needed to synthesize a specific MOF. Though current research on this topic is still in the early stages, it has seen a lot of interest and is based on the recent development of several databases of experimental MOF synthesis information. Such databases are assembled by application of text- and data-mining methods to the published scientific literature, including both journal articles and deposited crystal structures, through the use of either natural language processing (NLP) techniques (such as in the SynMOF⁴³ and DigiMOF⁴⁴ databases) or Large Language Models (LLM, as in the case of MOF-ChemUnity).⁴⁵

As we have seen, the computational determination of the experimental feasibility, or synthesizability, of hypothetical MOF structures is still a widely open challenge. Several approaches have been put forward, either relying on the evaluation of frameworks' thermodynamic and mechanical stability, or using data-driven methods to identify the similarity of a proposed structure to previously synthesized materials. These promising methodologies will no doubt be extended and complemented to get closer to a complete solution, and we seem to be at a pivotal moment for this important problem.

One of the active avenues of research is to broaden the existing criteria for stability. In addition to relying on thermodynamic and mechanical considerations, works have proposed to evaluate the thermal stability of framework materials, as well as stability upon activation of the as-synthesized material.³⁴ Going in this direction, the Kulik group has performed data mining of the published literature, through natural language processing and image analysis, to create data sets of solvent-removal stability measures, thermal degradation temperatures, as well as information on stability in water and in acidic conditions.^{46,47} They then used these new data sets to train machine-learning predictors for chemical robustness of MOF frameworks, with a stricter evaluation of stability that was not accessible before. It may also shift the discussion somewhat from the question of "synthesizability" to that of "usefulness": if a nanoporous material can be synthesized but cannot be activated or is not stable in mild conditions, what good is it as a candidate for applications? It certainly limits the range of usability, for example, to processes that do not require porosity or that can be designed to work around air- or water-sensitivity.

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Notes

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REFERENCES

- (1) Wilmer, C. E.; Leaf, M.; Lee, C. Y.; Farha, O. K.; Hauser, B. G.; Hupp, J. T.; Snurr, R. Q. Large-scale screening of hypothetical metal-organic frameworks. *Nat. Chem.* **2011**, *4*, 83–89.
- (2) Addicoat, M. A.; Couprie, D. E.; Heine, T. AuToGraFS: Automatic Topological Generator for Framework Structures. *J. Phys. Chem. A* **2014**, *118*, 9607–9614.
- (3) Colón, Y. J.; Gómez-Gualdrón, D. A.; Snurr, R. Q. Topologically Guided, Automated Construction of Metal–Organic Frameworks and Their Evaluation for Energy-Related Applications. *Cryst. Growth Des.* **2017**, *17*, 5801–5810.
- (4) Anderson, R.; Gómez-Gualdrón, D. A. Increasing topological diversity during computational "synthesis" of porous crystals: how and why. *CrystEngComm* **2019**, *21*, 1653–1665.
- (5) De Breuck, P.-P.; Wang, H.-C.; Rignanese, G.-M.; Botti, S.; Marques, M. A. L. Generative AI for crystal structures: a review. *npj Comput. Mater.* **2025**, *11*, 370.
- (6) Duan, C.; Nandy, A.; Chand Pal, S.; Yang, X.; Gao, W.; Du, Y.; Kraß, H.; Kang, Y.; Bernales, V.; Ye, Z.; et al. The rise of generative AI for metal-organic framework design and synthesis. *Matter* **2026**, *9*, 102748.
- (7) Ren, E.; Guilbaud, P.; Coudert, F.-X. High-throughput computational screening of nanoporous materials in targeted applications. *Digit. Discov.* **2022**, *1*, 355–374.
- (8) Gibaldi, M.; Kapeliukha, A.; White, A.; Luo, J.; Mayo, R. A.; Burner, J.; Woo, T. K. MOSAEC-DB: a comprehensive database of

experimental metal–organic frameworks with verified chemical accuracy suitable for molecular simulations. *Chem. Sci.* **2025**, *16*, 4085–4100.

(9) Tolborg, K.; Klarbring, J.; Ganose, A. M.; Walsh, A. Free energy predictions for crystal stability and synthesizability. *Digit. Discov.* **2022**, *1*, 586–595.

(10) Wu, X.; Jiang, J. Interrogating the synthetic likelihood of metal–organic frameworks: a digital discovery perspective. *Chem. Sci.* **2026**, *17*, 12635–12646.

(11) Akimbekov, Z.; Katsenis, A. D.; Nagabhushana, G. P.; Ayoub, G.; Arhangel'skii, M.; Morris, A. J.; Friščić, T.; Navrotsky, A. Experimental and Theoretical Evaluation of the Stability of True MOF Polymorphs Explains Their Mechanochemical Interconversions. *J. Am. Chem. Soc.* **2017**, *139*, 7952–7957.

(12) Cheetham, A. K.; Kieslich, G.; Yeung, H. H.-M. Thermodynamic and Kinetic Effects in the Crystallization of Metal–Organic Frameworks. *Acc. Chem. Res.* **2018**, *51*, 659–667.

(13) Anderson, R.; Gómez-Gualdrón, D. A. Large-Scale Free Energy Calculations on a Computational Metal–Organic Frameworks Database: Toward Synthetic Likelihood Predictions. *Chem. Mater.* **2020**, *32*, 8106–8119.

(14) Livas, C. G.; Trikalitis, P. N.; Froudakis, G. E. MOFSynth: A Computational Tool toward Synthetic Likelihood Predictions of MOFs. *J. Chem. Inf. Model.* **2024**, *64*, 8193–8200.

(15) Wu, X.; Zheng, R.; Liu, Q.; Jiang, J. Digital Discovery of Synthesizable Metal–Organic Frameworks via Molecular Dynamics-Informed, High-Fidelity Deep Learning. *Adv. Funct. Mater.* **2025**, *36*, e19565.

(16) Hollmann, N.; Müller, S.; Purucker, L.; Krishnakumar, A.; Körfer, M.; Hoo, S. B.; Schirmeister, R. T.; Hutter, F. Accurate predictions on small data with a tabular foundation model. *Nature* **2025**, *637*, 319–326.

(17) Niyongabo Rubungo, A.; Fajardo-Rojas, F.; Gómez-Gualdrón, D. A.; Dieng, A. B. Highly Accurate and Fast Prediction of MOF Free Energy via Machine Learning. *J. Am. Chem. Soc.* **2025**, *147*, 48035–48045.

(18) Dallmann, B.; Saha, A.; Rosen, A. S. Predicting the Thermodynamic Limits of Metal–Organic Framework Metastability. *J. Am. Chem. Soc.* **2026**, *148*, 19487–19501.

(19) Boström, H. L. B.; Goodwin, A. L. Hybrid Perovskites, Metal–Organic Frameworks, and Beyond: Unconventional Degrees of Freedom in Molecular Frameworks. *Acc. Chem. Res.* **2021**, *54*, 1288–1297.

(20) Bartel, C. J. Review of computational approaches to predict the thermodynamic stability of inorganic solids. *J. Mater. Sci.* **2022**, *57*, 10475–10498.

(21) Sun, W.; Dacek, S. T.; Ong, S. P.; Hautier, G.; Jain, A.; Richards, W. D.; Gamst, A. C.; Persson, K. A.; Ceder, G. The thermodynamic scale of inorganic crystalline metastability. *Sci. Adv.* **2016**, *2*, e1600225.

(22) Horton, M. K.; Huck, P.; Yang, R. X.; Munro, J. M.; Dwaraknath, S.; Ganose, A. M.; Kingsbury, R. S.; Wen, M.; Shen, J. X.; Mathis, T. S.; et al. Accelerated data-driven materials science with the Materials Project. *Nat. Mater.* **2025**, *24*, 1522–1532.

(23) Rieth, A. J.; Wright, A. M.; Dincă, M. Kinetic stability of metal–organic frameworks for corrosive and coordinating gas capture. *Nat. Rev. Mater.* **2019**, *4*, 708–725.

(24) Gálvez-Llompарт, M.; Gálvez, J.; Rey, F.; Sastre, G. Identification of New Templates for the Synthesis of BEA, BEC, and ISV Zeolites Using Molecular Topology and Monte Carlo Techniques. *J. Chem. Inf. Model.* **2020**, *60*, 2819–2829.

(25) Schwalbe-Koda, D.; Kwon, S.; Paris, C.; Bello-Jurado, E.; Jensen, Z.; Olivetti, E.; Willhammar, T.; Corma, A.; Román-Leshkov, Y.; Moliner, M.; et al. A priori control of zeolite phase competition and intergrowth with high-throughput simulations. *Science* **2021**, *374*, 308–315.

(26) Fajardo-Rojas, F.; Anderson, R.; Ardila, K.; Pak, A. J.; Gómez-Gualdrón, D. A. Interactions of Common Synthesis Solvents with MOFs Studied via Free Energies of Solvation: Implications on Stability and Polymorph Selection. *Chem. Mater.* **2026**, *38*, 607–618.

(27) Livas, C. G.; Klontzas, E.; Trikalitis, P. N.; Froudakis, G. E. MOFSynth-ADV: An Open-Source Engine for Synthesizability Evaluation of Metal–Organic Frameworks. *J. Chem. Inf. Model.* **2026**, *66*, 5040–5045.

(28) Bannwarth, C.; Caldeweyher, E.; Ehlert, S.; Hansen, A.; Pracht, P.; Seibert, J.; Spicher, S.; Grimme, S. Extended tight-binding quantum chemistry methods. *Wiley Interdiscip. Rev. Comput. Mol. Sci.* **2020**, *11*, e1493.

(29) Jacobs, R.; Morgan, D.; Attarian, S.; Meng, J.; Shen, C.; Wu, Z.; Xie, C. Y.; Yang, J. H.; Artrith, N.; Blaiszik, B.; et al. A practical guide to machine learning interatomic potentials – Status and future. *Curr. Opin. Solid State Mater. Sci.* **2025**, *35*, 101214.

(30) Coudert, F.-X. Systematic investigation of the mechanical properties of pure silica zeolites: stiffness, anisotropy, and negative linear compressibility. *Phys. Chem. Chem. Phys.* **2013**, *15*, 16012.

(31) Lee, S. J.; Doussot, C.; Baux, A.; Liu, L.; Jameson, G. B.; Richardson, C.; Pak, J. J.; Trouselet, F.; Coudert, F.-X.; Telfer, S. G. Multicomponent Metal–Organic Frameworks as Defect-Tolerant Materials. *Chem. Mater.* **2015**, *28*, 368–375.

(32) Coudert, F.-X.; Evans, J. D. Nanoscale metamaterials: Meta-MOFs and framework materials with anomalous behavior. *Coord. Chem. Rev.* **2019**, *388*, 48–62.

(33) Rogge, S. M. J.; Waroquier, M.; Van Speybroeck, V. Reliably Modeling the Mechanical Stability of Rigid and Flexible Metal–Organic Frameworks. *Acc. Chem. Res.* **2017**, *51*, 138–148.

(34) Mohamed, S. A.; Zhao, D.; Jiang, J. Integrating stability metrics with high-throughput computational screening of metal–organic frameworks for CO₂ capture. *Commun. Mater.* **2023**, *4*, 79.

(35) Moghadam, P. Z.; Rogge, S. M.; Li, A.; Chow, C.-M.; Wieme, J.; Moharrami, N.; Aragones-Anglada, M.; Conduit, G.; Gomez-Gualdrón, D. A.; Van Speybroeck, V.; et al. Structure-Mechanical Stability Relations of Metal–Organic Frameworks via Machine Learning. *Matter* **2019**, *1*, 219–234.

(36) Gaillac, R.; Chibani, S.; Coudert, F.-X. Speeding Up Discovery of Auxetic Zeolite Frameworks by Machine Learning. *Chem. Mater.* **2020**, *32*, 2653–2663.

(37) Lee, S.; Jeong, H.; Jung, S.; Kim, Y.; Cho, E.; Nam, J.; ChangMo Yang, D.; Shin, D. Y.; Lee, J.-H.; Oh, H.; et al. Data-Driven Search Algorithm for Discovery of Synthesizable Zeolitic Imidazolate Frameworks. *JACS Au* **2025**, *5*, 1460–1470.

(38) Helfrecht, B. A.; Pireddu, G.; Semino, R.; Auerbach, S. M.; Ceriotti, M. Ranking the synthesizability of hypothetical zeolites with the sorting hat. *Digit. Discov.* **2022**, *1*, 779–789.

(39) Pophale, R.; Cheeseman, P. A.; Deem, M. W. A database of new zeolite-like materials. *Phys. Chem. Chem. Phys.* **2011**, *13*, 12407.

(40) Bartók, A. P.; Kondor, R.; Csányi, G. On representing chemical environments. *Phys. Rev. B* **2013**, *87*, 219902.

(41) Zhao, G.; Brabson, L. M.; Chheda, S.; Huang, J.; Kim, H.; Liu, K.; Mochida, K.; Pham, T. D.; Prerna; Terrones, G. G.; et al. CoRE MOF DB: A curated experimental metal-organic framework database with machine-learned properties for integrated material-process screening. *Matter* **2025**, *8*, 102140.

(42) Zhang, C.; Antypov, D.; Rosseinsky, M. J.; Dyer, M. S. Accelerating metal–organic framework discovery via synthesizability prediction: the MFD evaluation method for one-class classification models. *Digit. Discov.* **2024**, *3*, 2509–2522.

(43) Luo, Y.; Bag, S.; Zaremba, O.; Cierpka, A.; Andreo, J.; Wuttke, S.; Friederich, P.; Tsotsalas, M. MOF Synthesis Prediction Enabled by Automatic Data Mining and Machine Learning. *Angew. Chem., Int. Ed.* **2022**, *61*, e202200242.

(44) Glasby, L. T.; Gubsch, K.; Bence, R.; Oktavian, R.; Isoko, K.; Moosavi, S. M.; Cordiner, J. L.; Cole, J. C.; Moghadam, P. Z. DigiMOF: A Database of Metal–Organic Framework Synthesis Information Generated via Text Mining. *Chem. Mater.* **2023**, *35*, 4510–4524.

(45) Pruyn, T. M.; Aswad, A.; Khan, S. T.; Huang, J.; Black, R.; Moosavi, S. M. MOF-ChemUnity: Literature-Informed Large

Language Models for Metal–Organic Framework Research. *J. Am. Chem. Soc.* **2025**, *147*, 43474–43486.

(46) Nandy, A.; Duan, C.; Kulik, H. J. Using Machine Learning and Data Mining to Leverage Community Knowledge for the Engineering of Stable Metal–Organic Frameworks. *J. Am. Chem. Soc.* **2021**, *143*, 17535–17547.

(47) Terrones, G. G.; Huang, S.-P.; Rivera, M. P.; Yue, S.; Hernandez, A.; Kulik, H. J. Metal–Organic Framework Stability in Water and Harsh Environments from Data-Driven Models Trained on the Diverse WS24 Data Set. *J. Am. Chem. Soc.* **2024**, *146*, 20333–20348.