Research Highlight | Open Access

AI Agent

Zhang *et al. AI Agent* **2026**, *2*, 15 **DOI:**10.20517/aiagent.2026.25

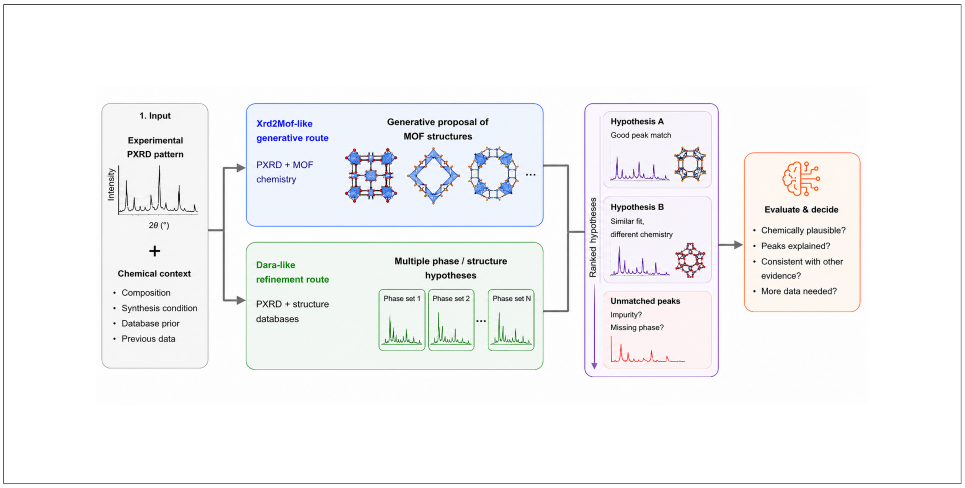
Decoding MOF structures from powder diffraction with generative AI

Linda Zhang[1,2], **Cheng Li**[3]

Citation: Zhang, L.; Li, C. Decoding MOF structures from powder diffraction with generative AI. *AI Agent* **2026**, *2*, 15. https://dx.doi.org/10.20517/aiagent.2026.25

Received: 11 Jun 2026
First Decision: 6 Jul 2026
Revised: 13 Jul 2026
Accepted: 17 Jul 2026
Published: 27 Jul 2026

Academic Editor: Aloysius Soon
Copy Editor: Tong Wang
Production Editor: Tong Wang



MAIN TEXT

Powder X-ray diffraction (PXRD) is a workhorse technique for metal-organic framework (MOF) characterization and often the first structural checkpoint after synthesis. In high-throughput MOF discovery, this reliance creates a bottleneck: data collection is fast and readily automated, but structural interpretation remains slow and expert-dependent. Single-crystal X-ray diffraction (SC-XRD) remains the gold standard for complete structure determination, yet many exploratory MOF reactions yield only microcrystalline powders, mixtures, flexible phases, defective materials, or crystals too small or unstable for SC-XRD. The difficulty is not merely poor data quality. MOF structures are large, topologically diverse, and combinatorially vast[1]. Metal-node positions and unit-cell geometry dominate many primary PXRD peaks, whereas organic linkers often contribute weaker, higher-angle features while carrying much of the chemistry relevant to gas storage, isotope separation, and catalysis. Peak overlap, preferred orientation, framework flexibility, guest contributions, and impurity phases further compress a complex three-dimensional problem into an ambiguous one-dimensional signal. The challenge for an AI agent is therefore not

[1]Frontier Research Institute for Interdisciplinary Sciences, Tohoku University, Sendai 980-0845, Japan.
[2]Advanced Institute for Materials Research (WPI-AIMR), Tohoku University, Sendai 980-8577, Japan.
[3]Spallation Neutron Source, Oak Ridge National Laboratory, Oak Ridge, TN 37830, United States.

Correspondence to: Dr. Linda Zhang, Frontier Research Institute for Interdisciplinary Sciences, Tohoku University, Sendai 980-0845, Japan. E-mail: linda.zhang.a3@tohoku.ac.jp

simply to assign a pattern, but to generate plausible structural hypotheses, expose uncertainty, and decide what evidence is still missing. Feng *et al*. now report Xrd2Mof, a generative AI model that moves MOF PXRD interpretation toward this agentic regime[2].

The central insight of Xrd2Mof is a physically motivated coarse-graining strategy. Rather than reconstructing full atomic-resolution structures directly from PXRD patterns, the model retains metal nodes as explicit three-dimensional coordinates while reducing organic linkers to centroids. This aligns the representation with diffraction physics: low-angle MOF peaks are strongly influenced by heavy-metal positions and lattice parameters, while linker-level details are often encoded in weaker high-angle features that are more easily obscured in laboratory data. This reduced representation preserves framework-level topology while making the generative problem tractable. Xrd2Mof combines multimodal feature extraction from PXRD, metal chemistry, and linker information with a diffusion model related to MOFdiff[3]. The learned embedding connects a one-dimensional diffraction pattern to chemically conditioned structural representations rather than treating PXRD as an isolated image-classification problem. Charge-neutrality constraints and linker SMILES strings guide the number of connection points, which are then matched to a database of approximately 400,000 linker building blocks[2]. The assembled structures are relaxed and ranked against the input PXRD pattern. Figure 1 summarizes this workflow, from multimodal encoding and coarse-grained generation to building-block assembly and structural relaxation.

The reported performance is striking: on approximately 10,000 CSD-derived MOFs, Xrd2Mof achieves top-10 success rates of 93.4% for single-linker and 96.2% for dual-linker frameworks[2]. The original study suggests that the strong dual-linker performance may be related to richer structural degrees of freedom available to the model; this interpretation should be viewed as model-specific rather than a general mathematical property of generative networks. Grad-CAM analysis indicates that the model primarily attends low-angle framework-diagnostic peaks, suggesting that it uses physically meaningful diffraction features rather than relying solely on statistical shortcuts. The experimentally measured ALICEE pattern, which contains offsets and background contributions absent from ideal simulated data, provides an encouraging first test beyond the training distribution. These results make Xrd2Mof important not because it replaces crystallographers, but because it can propose ranked structural hypotheses quickly enough to influence an automated discovery workflow.

A complementary perspective is offered by Dara, the data-driven automated Rietveld analysis workflow reported by Fei *et al.*[4]. Whereas Xrd2Mof addresses MOF-specific structure generation from known chemical inputs, Dara tackles phase identification and refinement in complex multicomponent inorganic patterns. It performs an exhaustive tree search over candidate phase combinations from structural databases, evaluates each node by peak matching and Rietveld refinement, groups isostructural alternatives by diffraction similarity, and returns all solutions with comparable fit quality along with diagnostics for unmatched peaks. This is epistemically important: in many PXRD problems, several chemically distinct models can explain the observable peaks almost equally well. The Dara workflow is shown in Figure 2. Dara has already been deployed at A-Lab, processing more than 2,400 experimental patterns with a median runtime of 88.9 s[4,5]. Xrd2Mof contributes generative structural imagination; Dara contributes disciplined hypothesis testing.

This contrast is useful because earlier machine-learning methods had already accelerated X-ray diffraction (XRD) classification and multiphase interpretation[6,7], but many workflows still reduce ambiguity to a single label or confidence score. Xrd2Mof and Dara instead preserve ambiguity as a first-class output. Multiple structures or phase combinations are returned, ranked, and accompanied by diagnostics indicating whether the present evidence is sufficient. Table 1 summarizes the boundary between Xrd2Mof and Dara and their

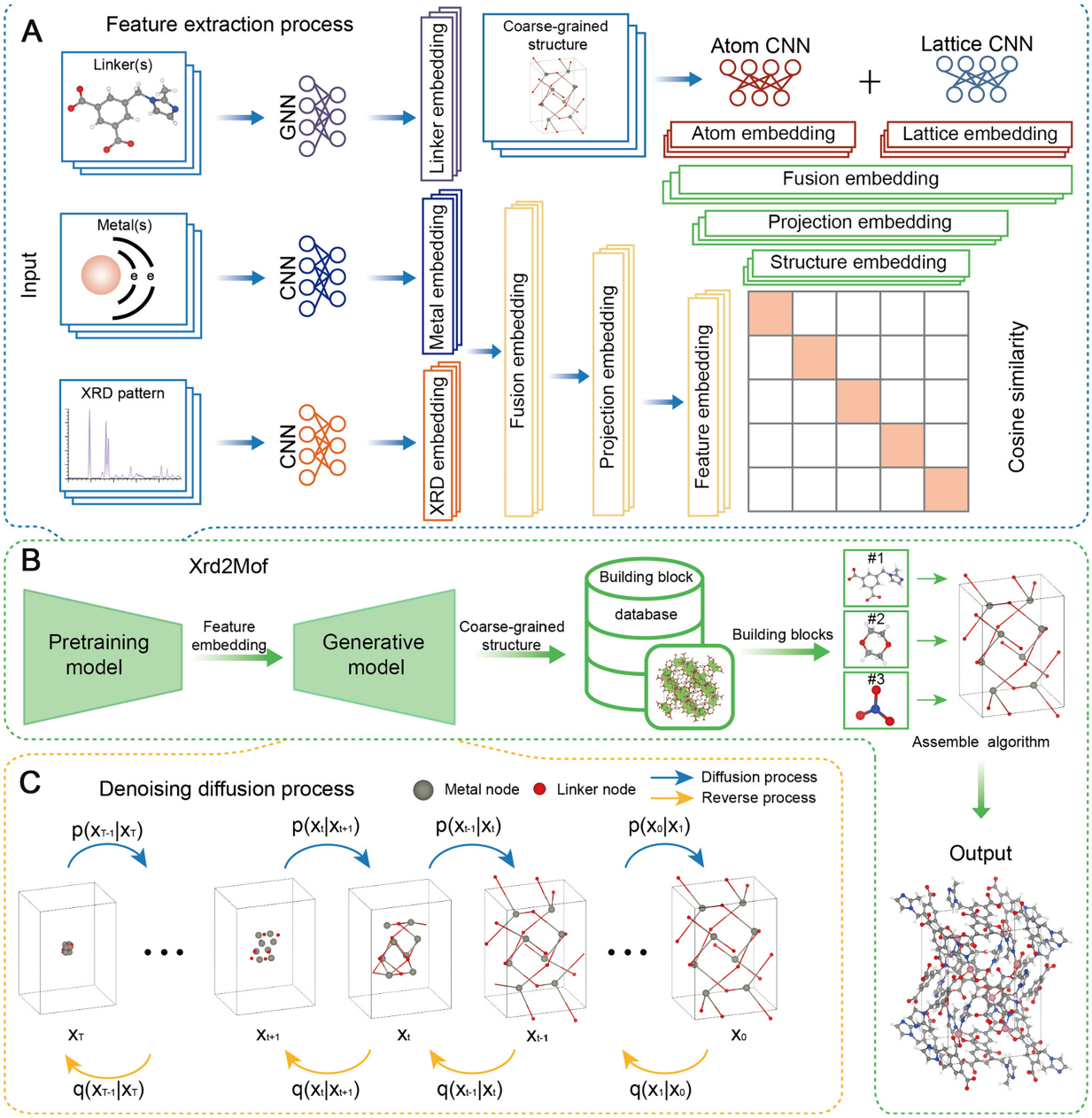


Figure 1. Architecture and workflow of Xrd2Mof for generative interpretation of metal-organic framework structures from powder X-ray diffraction patterns. (A) Pretrained multimodal feature-extraction module. Simulated PXRD patterns, metal-node information, and organic-linker information are processed by dedicated neural networks, fused, and projected into feature vectors for comparison with coarse-grained structural representations. After pretraining, the feature-extraction module is frozen; (B) Overall Xrd2Mof workflow. The extracted feature vectors guide the diffusion-based generation of coarse-grained MOF candidates. Corresponding building blocks are then retrieved from a database, assembled into atomistic structures, and optimized using a force-field method. Multiple candidate structures are generated for subsequent evaluation; (C) Conditional diffusion model for coarse-grained structure generation. During training, node types and valences are initialized using chemical prior knowledge and iteratively refined under the guidance of the extracted feature vectors and diffusion time steps; during inference, the reverse diffusion process generates candidate structures. Reproduced with permission from reference[2]. Copyright 2026 American Chemical Society. PXRD: Powder X-ray diffraction; MOF: metal-organic framework; CNN: convolutional neural network; GNN: graph neural network.

complementary roles in an agentic PXRD workflow. An orchestration agent receiving these outputs could filter candidates by synthesis chemistry, charge balance, adsorption or stability predictions, and prior measurements. If uncertainty remains high, the agent could request composition-sensitive elemental mapping by scanning electron microscopy coupled with energy-dispersive X-ray spectroscopy (SEM-EDS)[8], synchrotron or neutron diffraction, spectroscopy, pair distribution function analysis, or gas-adsorption measurements, depending on which ambiguity matters most.

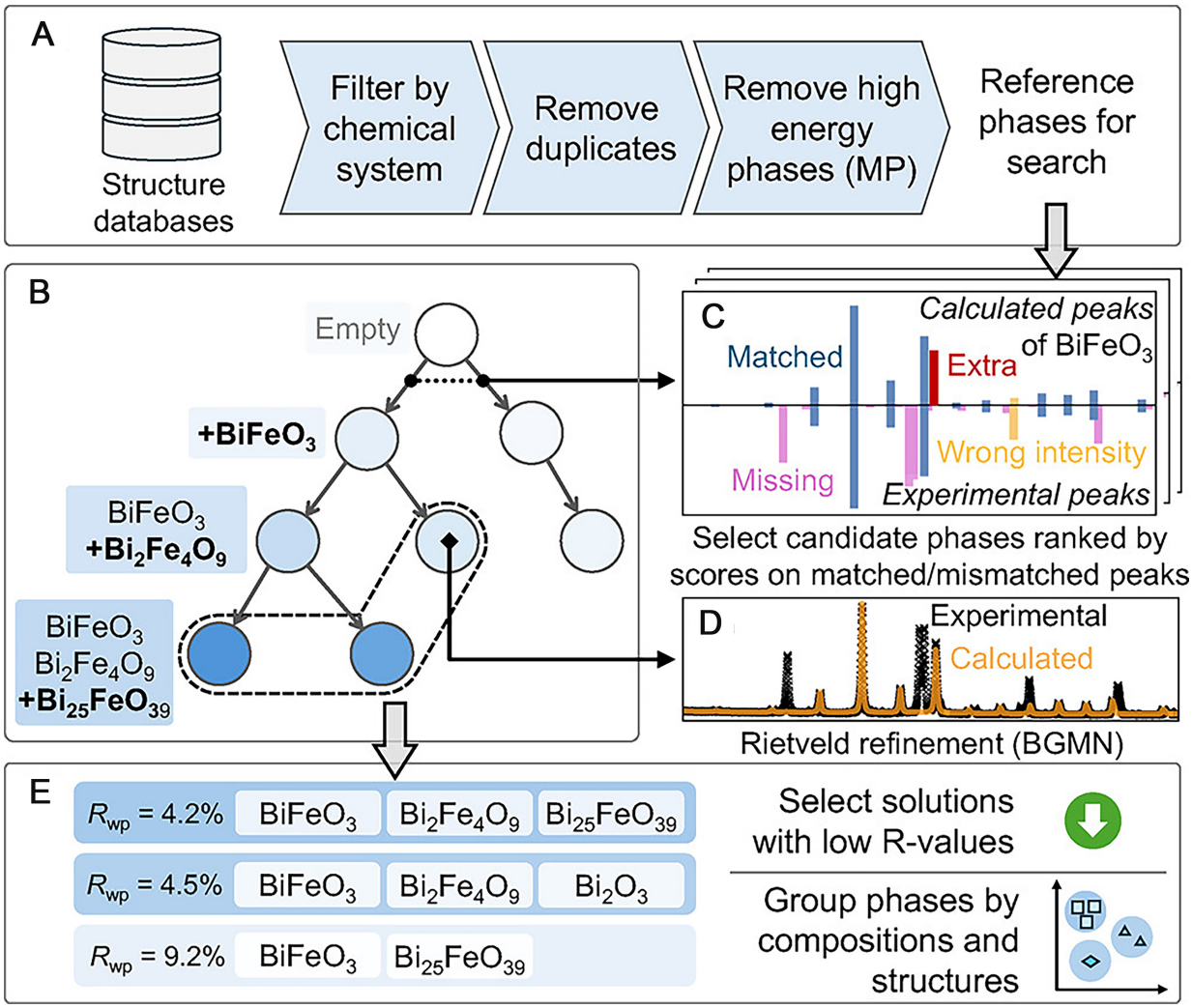


Figure 2. Overview of powder X-ray diffraction phase analysis using Dara. (A) Preprocessing workflow for selecting reference phases from structural databases. Candidate phases within the chemical system of the input diffraction pattern are retained, duplicate structures are removed based on composition and space group, and high-energy phases are excluded using thermodynamic data from the Materials Project; (B) Search tree in which each node represents a phase combination and each directed edge represents the addition of one phase. Node color indicates the weighted-profile residual (R_{wp}), with darker colors corresponding to lower values and therefore better fits; (C) Peak-matching algorithm used to identify phases that can account for the remaining unmatched peaks, thereby pruning unlikely candidates and reducing computational cost; (D) Rietveld refinement of the selected phases using BGMN. Black crosses represent the experimental diffraction pattern, and the orange line represents the calculated pattern; (E) Candidate solutions extracted from the search tree, ranked by R-values and grouped according to composition and structure; solutions with excessively high R-values are excluded. Reproduced unchanged from reference[4] under the Creative Commons CC BY-NC-ND 4.0 license. Dara: Data-driven automated Rietveld analysis; XRD: X-ray diffraction; PXRD: powder X-ray diffraction; COD: Crystallography Open Database; MP: Materials Project.

In the meantime, limitations remain. For Xrd2Mof, the train-test domain gap is central: simulated PXRD patterns do not fully capture peak broadening, preferred orientation, background, guest contributions, defects, or breathing transitions in laboratory data. Systematic benchmarks across experimental MOF patterns remain limited, and generalization to previously unseen MOF families, highly defective frameworks, or materials underrepresented in training databases is still unproven. The method also assumes that the linker supplied as input survives synthesis intact; unexpected *in situ* functionalization, solvolysis, or changes in protonation state would break this assumption. For Dara, the ceiling is database coverage: phases absent

Table 1. Boundary and synergy between Xrd2Mof and Dara

Dimension	Xrd2Mof	Dara
Target problem	MOF structure proposal from PXRD and known chemistry	Phase identification/refinement from multiphase PXRD
Prior knowledge	Metal and linker information; MOF-focused representation	Candidate phases from structural databases
Output	Ranked candidate MOF structures	Multiple refined phase hypotheses and unmatched-peak diagnostics
Strength	Generative structural imagination	Disciplined hypothesis testing
Main bottleneck	Simulated-to-experimental gap; unseen/defective/flexible MOFs	Database coverage; unresolved ambiguity
Agentic role	Propose structures for downstream checking	Test and refine competing hypotheses

MOF: Metal-organic framework; PXRD: powder X-ray diffraction.

from reference databases, disordered materials, and poorly represented metastable structures cannot be confidently identified. More broadly, PXRD is not always the decisive experiment for porous materials, where light atoms, guest molecules, partial occupancy, local disorder, framework dynamics, or magnetic order may control structure-function relationships. A useful AI crystallographer should therefore know when the current pattern is enough and when another measurement would reduce uncertainty more efficiently than another round of fitting.

The progress represented by Xrd2Mof and Dara is therefore not merely an incremental improvement to XRD software. It signals a shift from automated pattern matching toward evidence-aware structural reasoning. A closed-loop MOF laboratory could connect robotic synthesis, PXRD collection, generative structure proposal, multi-hypothesis refinement, property prediction, and targeted follow-up experiments, building on progress in self-driving laboratories[9]. The difficult problem is not prediction alone, but orchestration across synthesis conditions, structural hypotheses, properties, and feedback. AI in materials characterization should become more scientific, not merely more automated: it should manage evidence, uncertainty, and alternative hypotheses well enough to decide the next experiment.

DECLARATIONS

Authors' contributions

Conception and design of the article, literature analysis, and manuscript writing: Zhang, L.; Li, C.
Both authors read and approved the final manuscript.

Availability of data and materials

Not applicable.

AI and AI-assisted tools statement

During the preparation of this manuscript, the AI tool OpenAI ChatGPT (version GPT-5.5, released 2026-4-24) was used solely for language polishing. The tool did not influence the study design, data collection, analysis, interpretation, or the scientific content of the work. Both authors take full responsibility for the accuracy, integrity, and final content of the manuscript.

Financial support and sponsorship

None.

Conflicts of interest

Both authors declared that there are no conflicts of interest.

Ethical approval and consent to participate

Not applicable.

Consent for publication

Not applicable.

Copyright

REFERENCES

1. Furukawa, H.; Cordova, K. E.; O'keeffe, M.; Yaghi, O. M. The chemistry and applications of metal-organic frameworks. *Science* **2013**, *341*, 1230444. DOI PubMed
2. Feng, B.; Wang, B.; Lv, L.; et al. Interpreting X-ray diffraction patterns of metal-organic frameworks via generative artificial intelligence. *J. Am. Chem. Soc.* **2025**, *148*, 869-78. DOI PubMed
3. Fu, X.; Xie, T.; Rosen, A. S.; Jaakkola, T.; Smith, J. MOFdiff: coarse-grained diffusion for metal-organic framework design. *arXiv* **2023**, arXiv:2310.10732. Available online: https://arxiv.org/abs/2310.10732 (accessed 5 June 2026).
4. Fei, Y.; Mcdermott, M. J.; Rom, C. L.; Wang, S.; Ceder, G. Dara: automated multiple-hypothesis phase identification and refinement from powder X-ray diffraction. *Chem. Mater.* **2026**, *38*, 1364-76. DOI PubMed PMC
5. Szymanski, N. J.; Rendy, B.; Fei, Y.; et al. An autonomous laboratory for the accelerated synthesis of inorganic materials. *Nature* **2023**, *624*, 86-91. DOI PubMed PMC
6. Oviedo, F.; Ren, Z.; Sun, S.; et al. Fast and interpretable classification of small X-ray diffraction datasets using data augmentation and deep neural networks. *npj. Comput. Mater.* **2019**, *5*, 60. DOI
7. Szymanski, N. J.; Bartel, C. J.; Zeng, Y.; Tu, Q.; Ceder, G. Probabilistic deep learning approach to automate the interpretation of multi-phase diffraction spectra. *Chem. Mater.* **2021**, *33*, 4204-15. DOI
8. Newbury, D. E.; Ritchie, N. W. M. Is scanning electron microscopy/energy dispersive X-ray spectrometry (SEM/EDS) quantitative? *Scanning* **2013**, *35*, 141-68. DOI PubMed
9. Tom, G.; Schmid, S. P.; Baird, S. G.; et al. Self-driving laboratories for chemistry and materials science. *Chem. Rev.* **2024**, *124*, 9633-732. DOI PubMed PMC