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Topology-aware AI for porous materials: from structural representation to counterfactual testing and inverse design

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Perspective

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Abstract

Artificial intelligence is reshaping porous material design, but most workflows still compress complex void spaces into scalar descriptors that cannot uniquely specify transport pathways. This Perspective surveys the progression from adsorption-derived descriptors and pore-network models to persistent topology, geometric learning, digital twins and multimodal structural inference. It identifies a weakness: predictive accuracy rarely establishes that a model has learned connectivity. We position counterfactual topology twins—descriptor-matched structures with deliberately different networks—as a unifying stress test. Combined with grouped validation, calibrated uncertainty and realizability constraints, this framework could turn topology from a hidden correlate into a measurable and designable variable.

Introduction

Artificial intelligence (AI) has changed how materials are screened, optimized and increasingly proposed. Large databases, high-throughput simulation and modern learning algorithms can traverse chemical spaces that are inaccessible to intuition alone.[1] Porous materials are natural beneficiaries because their performance in separations, catalysis and electrochemical devices depends on a combination of factors including composition, pore geometry and operating conditions. Machine learning has already accelerated property prediction and candidate ranking across these systems.[2]

Yet porous materials also expose a basic limitation of data-driven design: a model cannot learn structural information that was never represented. Many datasets reduce porous materials' complex void space to surface area, pore volume, pore-size distribution, density and composition descriptors. Those variables remain indispensable, but they do not uniquely determine how pores communicate. Networks containing long channels, redundant cross-links, isolated closed pockets or restrictive throats can share similar scalar summaries but behave differently once matter moves through them.[3–6]

The field is responding along several fronts. At the same time, research on shortcut learning and cross-domain deployment has shown why a richer representation alone is not proof of generalization.[7–9] Image analysis and pore-network extraction retain spatial organization; topological data analysis summarizes multiscale structure; geometric learning operates directly on graphs or coordinates; digital twins connect stochastic morphology with transport; and multimodal inference combines complementary measurements.[4, 10–16] These developments are often discussed separately, although they confront the same question: which representation preserves the structural distinctions that control a process?

This Perspective first synthesizes that emerging landscape and its unresolved limitations. We then argue that the next step is not simply to add more complex descriptors, but to test whether a model is genuinely sensitive to connectivity. Counterfactual topology twins—pairs matched in conventional descriptors but deliberately separated in network organization—provide one way to perform that test.

The proposal is, therefore, positioned here as an auditing and design layer that can sit above several existing representations, rather than as a replacement for them.

The state of the art: how porous structure enters AI

Scalar descriptors remain the necessary baseline

Scalar descriptors are attractive because they are inexpensive, interpretable and available for many materials. Adsorption measurements provide surface area, pore volume and pore size distributions; elemental analysis and spectroscopy add composition and surface chemistry; and bulk measurements supply density, conductivity or mechanical response. Such variables support tabular models that can be trained on modest datasets and can reveal broad trends. They are also the only defensible starting point for asking whether a more elaborate representation adds value.[2, 3]

Their weakness is many-to-one compression. Distinct microstructures can produce similar isotherms or scalar summaries, and a pore size distribution does not state whether pores lie in series, in parallel or in disconnected regions. Geometrical disorder can shift confined phase behavior even when nominal pore sizes remain comparable.[5] Scalar models can, therefore, predict well within a synthesis family while failing when connectivity, disorder or operating conditions change. The limitation is not a defect in the algorithm, but a structural non-identifiability in the input.

Images and pore network models preserve spatial organization

Tomography, microscopy and voxelized simulations make connectivity visible over a finite field of view. Segmentation can be followed by skeletonization or pore network extraction, representing pore bodies as nodes and throats as edges. Open analysis tools have made this workflow increasingly reproducible.[4] Network models then calculate coordination, shortest paths, tortuosity, centrality, percolation and transport at a fraction of the cost of full-field simulation. They provide an interpretable bridge between morphology and performance.[3, 4]

That bridge is not neutral. Resolution, segmentation thresholds, boundary truncation and the rule used to define a throat all change the resulting graph. A small imaging volume can miss long-range paths; a skeleton can suppress pore shape; and two plausible extraction pipelines can give different topologies. Network statistics should, therefore, be treated as inferences with method-dependent uncertainty, not as direct observations. Retaining alternative reconstructions is often more informative than selecting one graph and forgetting how it was obtained.

Topology provides multiscale summaries

Topological data analysis offers a complementary form of compression. Persistent homology records the appearance and disappearance of connected components, loops and cavities as a filtration scale changes.[15] Persistence diagrams, landscapes or images can become machine learning features, while distances between diagrams provide measures of structural dissimilarity. Applications in amorphous solids and halide perovskites show that these summaries can recover structural organization missed by conventional features and sometimes improve transfer across held-out chemical groups.[12, 16]

Recent results in NPG Asia Materials strengthen the case for materials-relevant topology: persistent-homology analysis linked intermediate-range network disorder in $TiNb_2O_7$ to degradation of negative electrode performance.[10] The important lesson is not that persistent homology is universally superior. A topological feature is only meaningful relative to the point cloud, graph, filtration and length scale used to construct it. In transport problems, a mathematically persistent loop may be inaccessible to the moving species, while a short-lived bottleneck may dominate the observed response. Physical interpretation must guide the topology.

Geometric learning, hybrid physics and digital twins

Geometric and graph learning reduce the need to preselect a small set of statistics. Models can operate on atoms, pore bodies, throats, meshes or multiscale graphs and learn representations from local geometry and connectivity. Physics-inspired representations can encode symmetry and interactions while hybrid models combine learning with molecular simulation, pore network transport or continuum conservation laws.[14] These approaches are powerful when the training data span the relevant structural variation, but their flexibility also permits shortcut learning and makes graph construction part of the model rather than a harmless preprocessing choice.[7]

Digital twins extend the idea from representation to a computational counterpart of the material. A recent porous adsorption example combined stochastic microstructure generation, mathematical morphology and deep learning to reproduce adsorption behavior from basic porosity information.[11] Elsewhere, topology-based generative models have enabled interpretable inverse design of catalytic active sites.[13] Together, these studies show a shift from predicting a property of a fixed structure toward generating plausible structures under target constraints. They also expose a central risk: a generated twin can match selected observables while remaining wrong in unmeasured connectivity.

Table 1 places these approaches on one continuum. No single representation dominates every task. Scalar models offer transparency and coverage, imaging offers local realism, network and topological models offer interpretable structure, geometric learning offers flexibility, and physics-informed digital twins offer a route to intervention. Active learning adds a principled way to choose the next calculation or experiment under uncertainty.[17] The unresolved need is a common test that asks whether each representation responds correctly when topology changes and conventional descriptors do not.

Table 1
Representation landscape for topology-aware porous materials AI

Approach	Structural object	Principal strength	Main blind spot
Scalar descriptors	Sorption, composition and bulk-property vectors	Low-data baselines, screening and interpretation	Cannot uniquely specify paths or connectivity
Images and voxels	Microscopy, tomography or simulated fields	Spatial morphology and local heterogeneity	Finite field of view; resolution and segmentation bias
Pore networks	Pore-body nodes and throat edges	Transport paths, bottlenecks and percolation	Extraction rules simplify shape and alter topology
Topological summaries	Graphs, point clouds or filtrations	Multiscale components, loops and cavities	Meaning depends on filtration and process scale
Geometric learning	Atoms, graphs, meshes or multiscale structures	Learned local and non-local representations	Data demand, shortcuts and opaque sensitivities
Hybrid and digital twins	Generative structure plus physical simulation	Prediction, intervention and inverse design	Non-unique calibration and uncertain realizability

Characterization and the problem of identifiability

The representation landscape is inseparable from measurement. No experiment returns topology without interpretation. Imaging resolves spatial detail over a limited volume, scattering and sorption provide ensemble averages but require non-unique inversion, and nuclear magnetic resonance (NMR) constrains diffusion, relaxation and exchange while averaging over heterogeneous environments.[5, 6, 18–20] Treating any one technique as ground truth hides the assumptions that map an observable to a network.

Our previous work illustrates why those projections must be combined. Geometric disorder alters confined phase equilibria,[5] and comparisons of channel-like CMK-3 with hierarchically connected ST-CMK-3 show that two-dimensional exchange spectroscopy can resolve asymmetric exchange pathways that are not inferable from pore volume alone.[6] Pulsed-field-gradient NMR can constrain effective and anisotropic diffusion, relaxation measurements probe confinement and surface interaction, and exchange spectroscopy reports communication between environments.[18–20] None of these signals, by itself, specifies a unique three-dimensional graph.

A better formulation is a posterior distribution over networks that are consistent with all available observations. Alternative segmentations, graph constructions and model parameters can then be propagated into predictions. Active learning can select the next measurement that most reduces

disagreement among plausible structures.[17] This changes characterization from a final verification step into part of the learning loop and creates a natural role for multimodal data fusion and calibrated uncertainty.

The validation gap

The rapid expansion of structural representations has not been matched by equally discriminating validation. Random train–test splits remain common even when measurements share a precursor, synthesis route or parent structure. Closely related samples can consequently appear on both sides of the split, allowing recognition of a family to masquerade as generalization. Shortcut learning is especially difficult to detect when chemistry, pore size and topology change together.[7]

Domain shift exposes the problem more clearly. Latent representations can appear well aligned while failing to preserve target-relevant relationships, and deployment across electrochemical-material domains requires explicit auditing of transfer assumptions.[8, 9] For topology-aware AI, family-level holdouts, prospective tests and sensitivity to graph construction are, therefore, more informative than a marginal improvement in random-split error. A model should also be tested on the structural distinction it claims to have learned.

Current studies provide compelling examples of topology–property association, but association, prediction and intervention are different standards of evidence.[10–13] An interpretable topological feature may correlate with performance without being the operative transport variable. A geometric model may predict accurately while relying on chemistry. A digital twin may reproduce an isotherm while missing exchange routes. This gap motivates a controlled counterfactual test that can be applied across representation classes.

Counterfactual topology twins as a common stress test

Here, we use the term topology twins for a pair of porous structures, A and B, that are closely matched in conventional material descriptors but deliberately differ in one or more connectivity characteristics. For each structure i, x_i is the conventional scalar-descriptor vector, for example, surface area, pore volume, pore size distribution, composition and density. T_i is the chosen topology representation, for example, coordination statistics, tortuosity, dead-end fraction, bottleneck centrality, cycle structure or persistent-homology features. The quantity y_i is a measured or simulated process response, such as diffusivity, exchange rate, accessible capacity, permeability or catalytic turnover. Formally, structures A and B qualify as topology twins only when they satisfy the joint criterion $d_s(x_A, x_B) \leq \epsilon_s$ and $d_T(T_A, T_B) \geq \epsilon_T$, meaning that they are matched within a predefined tolerance in conventional descriptor space while remaining separated by at least a predefined amount in topology space. Here, d_s is a predefined distance measure and ϵ_s is the maximum tolerated mismatch, whereas d_T is the selected topological distance and ϵ_T is the minimum required topological contrast. Descriptor normalization,

variable weights, distance functions and both thresholds should be declared before the response is examined. The paired response is $\Delta y = y_B - y_A$, with the ordering of A and B fixed in advance. A topology-aware model should predict the sign and magnitude of Δy and provide an uncertainty interval with credible empirical coverage.[3–6]

This definition is deliberately representation-agnostic. A scalar model establishes whether matching is adequate; a pore network model supplies interpretable contrasts; persistent topology tests multiscale organization; a geometric model learns richer representations; and a hybrid model connects network edits to transport. Topology twins are, thus, an audit layer across the state of the art, not a competing descriptor. Their value lies in asking every model the same counterfactual question after familiar scalar cues have largely been removed, as illustrated in Fig. 1.

Computational pairs can be created by network rewiring, controlled throat deletion, loop insertion, channel segmentation or morphology-preserving operations that maintain pore volume and approximately maintain size statistics. Experimental pairs may be approached through templating, activation, post-synthetic linking, particle assembly or partial pore blocking. Useful contrasts include coordination number, percolating-path multiplicity, bottleneck centrality, tortuosity, cycle rank and persistence across relevant length scales.[3–5, 10, 15, 16]

The construction does not establish causality automatically. Its interpretation depends on matching quality, measurement error, absence of unmeasured chemical changes and relevance of the chosen scale. A strong study should, therefore, show that scalar-only models cannot reliably distinguish the pair, include null pairs with no intended topology contrast and test topology changes outside the process-relevant scale. Here, failure is informative, as it may show that the representation missed relevant connectivity, that the experiment did not identify it, or that topology was not decisive under the stated conditions.

From topology-aware prediction to inverse design

A model should not be trusted for inverse topology design merely because it predicts a conventional test set. It should first distinguish topology twins outside its training families, remain calibrated under alternative graph reconstructions and retain the predicted contrast when plausible disorder is introduced. Only then does it become reasonable to optimize connectivity itself.

The objective should be process-level rather than a graph statistic in isolation: accessible capacity at a specified charging time, catalytic turnover without product trapping, or selectivity subject to mechanical integrity. Shorter paths, wider throats and greater redundancy can trade against surface area, selectivity or stability, so multi-objective optimization is unavoidable. Generative models can propose topology-aware active sites and networks,[13] while digital twins can screen how morphology influences adsorption or transport.[11] Every proposal still requires filters for geometric realizability, synthesis plausibility and robustness to manufacturing variation.

We envisage a closed loop in which complementary measurements constrain a structural posterior; multiple representations are benchmarked; topology twins challenge the model; and feasible network edits are proposed for simulation or fabrication (Fig. 2). New evidence updates both the posterior and the next experiment. Active learning is valuable because the most informative material may not be the one with the highest predicted performance, but the one that resolves a persistent topology–performance ambiguity.[17]

A benchmark and reporting standard

A useful community benchmark would preserve more of the experimental record than a conventional descriptor table. It should contain raw structures or images, alternative network reconstructions, process conditions, uncertainty and provenance linking every parent to its twin. Computational pairs can provide scale, whereas experimentally realized pairs provide realism; the two should be labelled and evaluated separately. Reusable structures, protocols and software would enable comparison across laboratories and material classes.[2, 4, 8, 9, 11]

Evaluation should distinguish interpolation, family holdout, counterfactual ranking and prospective prediction. Alongside absolute error, studies should report directional accuracy for Δy, error in predicted Δy, pairwise ranking, calibration and interval coverage. Representation-ladder ablations—scalar, network, topological, geometric and hybrid—should use identical splits and data budgets. Model cards should document graph construction, leakage controls, uncertainty, computational cost and failure cases.

Table 2 proposes a minimum reporting standard. It is intentionally compact enough to be adopted across adsorption, separations, catalysis and electrochemical transport. The purpose is not to prescribe one topology, but to make claims comparable and falsifiable. Pairs for which topology produces no measurable response, or for which measurements cannot identify the network, should remain in the dataset rather than disappear as unhelpful results.

Table 2
Minimum reporting standard for topology-twin studies

Item	Minimum information
Twin definition	State parent–twin provenance, intervention and material family.
Matching tolerance	Report d_s, ϵ_s, matched variables, uncertainty and scalar-only discrimination.
Topology contrast	Define T, d_T, ϵ_T, graph construction, scale and filtration choices.
Process conditions	State temperature, pressure, composition, field, timescale and boundaries.
Validation split	Group twins, hold out complete families and reserve a prospective set.
Pairwise performance	Report sign accuracy, Δy error, ranking, calibration and interval coverage.
Controls and ablations	Include representation-ladder ablations, null pairs and off-scale changes.
Structural uncertainty	Propagate alternative reconstructions or posterior samples into predictions.
Reproducibility	Release structures, raw/processed data, code, seeds and protocols where possible.

Outlook: priorities for the field

The first priority is to define topology at the scale of the process. Atomic, mesoscopic and device-level graphs answer different questions, and the relevant scale can shift with probe molecule, electrolyte, temperature or operating time. A universal fingerprint is less plausible—and less useful—than a hierarchy of representations tied to explicit transport regimes.

The second priority is paired, multimodal data. Large, unpaired datasets will continue to support screening, but carefully designed contrasts are needed to identify what a model has learned. Imaging, sorption, scattering, NMR and transport should be acquired on the same materials with uncertainty and provenance intact.[5, 6, 18–20] The third priority is prospective validation across material families. Domain-shift audits should become part of model development, not an exercise performed after deployment.[8, 9]

The final priority is synthesis-aware intervention. The field should judge inverse design by whether it proposes changes that can be made, measured and shown to improve process-level performance under disorder. A topology-aware model that survives counterfactual tests but cannot produce a realizable structure remains diagnostically useful; one that also guides fabrication would turn connectivity from a hidden correlate into a controllable materials variable.

Conclusions

Porous materials AI is moving beyond scalar descriptor tables toward images, pore networks, persistent topology, geometric learning and digital twins. Each advance preserves a different part of structural information, yet none alone proves that a model has learned the connectivity relevant to transport. The field, therefore, needs validation objects that separate topology from the conventional cues with which it is normally entangled.

Counterfactual topology twins offer one such object. Positioned within the broader representation landscape, they provide a common stress test, support pairwise benchmarking and create a bridge from structural inference to inverse design. Their most important feature is that they can fail. That possibility keeps claims proportionate to the evidence and clarifies when topology must be measured, represented and designed—and when simpler descriptors are sufficient.

Declarations

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Contributions

H.R.N.B.E. developed the scope and central argument of the Perspective, selected and critically synthesized the literature, formulated the counterfactual topology twins framework and its proposed validation criteria, prepared the figures, wrote and revised the manuscript.

Competing interests

The author declares no competing interests.

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Data availability

No new datasets were generated or analyzed for this Perspective.

Use of generative artificial intelligence

OpenAI ChatGPT (version 5.6) was used to support language editing. The author independently developed and verified the scientific arguments, checked the accuracy and relevance of the references, critically revised all text, and accepts full responsibility for the submitted content.

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Figures

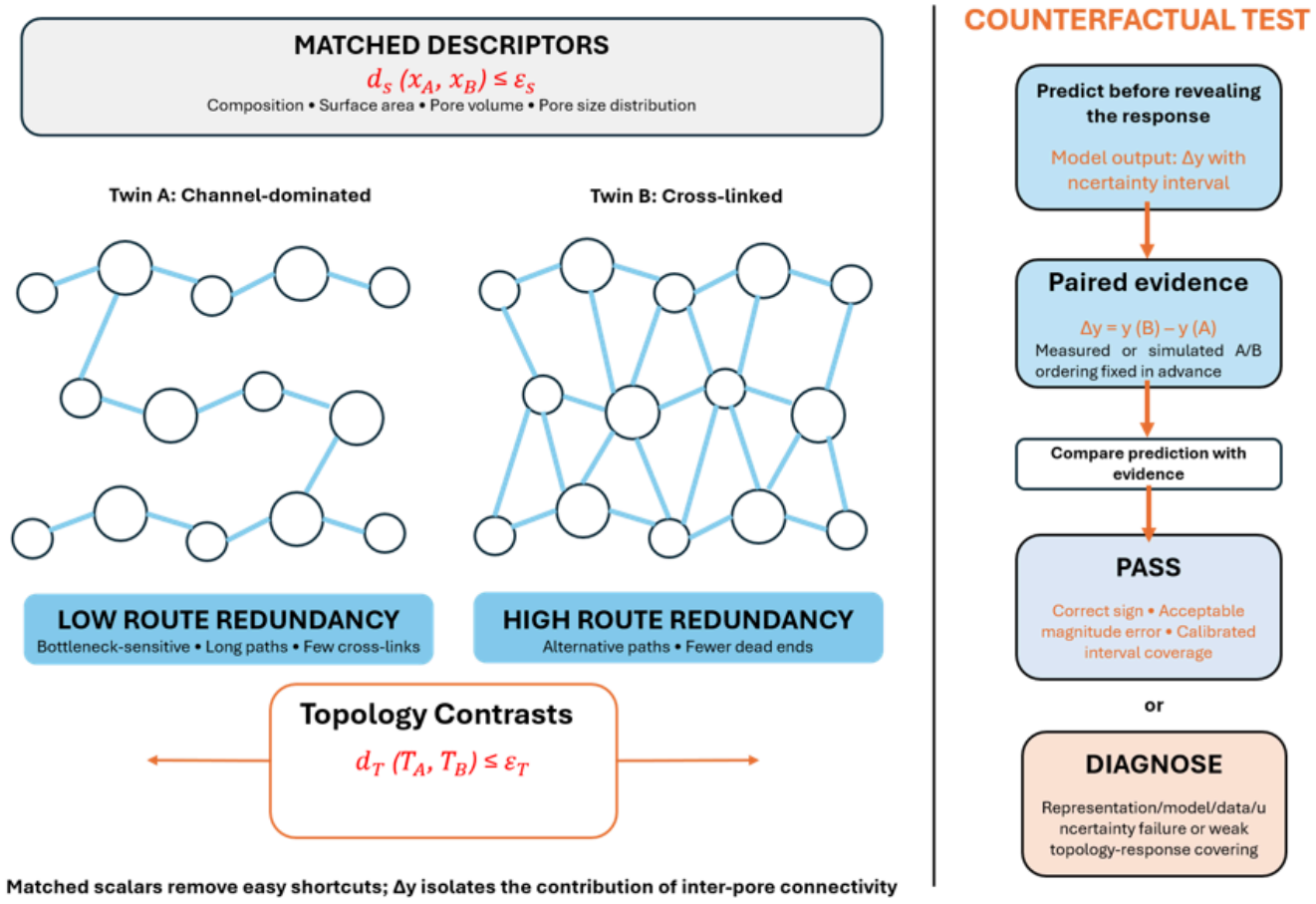


Figure 1

Counterfactual topology twins. Two porous networks are matched within declared tolerances for conventional scalar descriptors but differ in route redundancy, cross-linking and dead-end structure. Their paired transport response tests whether a model predicts the direction and magnitude of Δy after familiar scalar cues have been controlled.

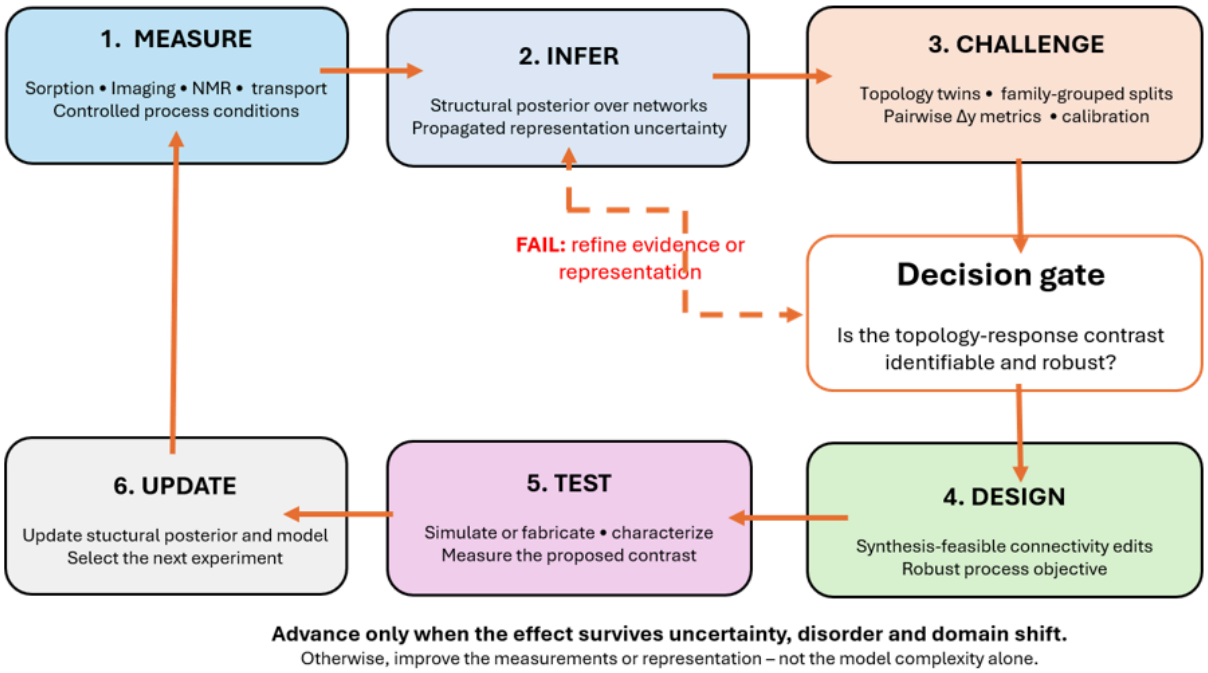


Figure 2

Closed-loop topology-aware materials AI. Complementary observations constrain structural representations; topology twins challenge models under grouped splits and pairwise metrics; feasible network edits are proposed under synthesis and robustness constraints; and new evidence updates the structural posterior and the next experiment.