Title: **Visualizing Uncertainty in Inverse Catalyst Design: Toward Robust Solutions for Energy and Critical Materials**

Peng Xu (pxu@ameslab.gov), Ames National Laboratory,

Lin Yan (linyan@iastate.edu), Liyi Li (liyili2@iastate.edu), Qi An (qan@iastate.edu), Iowa State University

Topic: **Optimization algorithms for inverse problems under uncertainty**

Challenge: A catalyst is a substance that accelerates chemical reactions or reduces the energy required to initiate them, without being consumed in the process. By lowering the energy barrier reactants must overcome, catalysts enable faster, more sustainable transformations. Beyond accelerating reactions, they often exhibit precise selectivity, steering pathways toward desired products while minimizing byproducts. Optimizing catalytic performance (activity, selectivity, and stability) is critical for many modern industrial processes, yet designing catalysts experimentally remains costly and complex. For instance, porous nanocatalysts depend on intricate variables such as the spatial distribution of active sites, pore geometry, functional group composition, and external conditions like temperature, pressure or solvent effects. These parameters create a vast, high-dimensional search space where only sparse regions yield high-performing candidates. While atomistic simulations and electronic structure theory have expanded predictive capabilities, the combinatorial explosion of variables makes systematic exploration impractical. This positions catalyst design as an inverse problem: identifying the optimal combination of atomic-scale properties, nanoscale morphology, and operational conditions to achieve target performance metrics, guided by computational models and data-driven strategies. However, catalyst optimization is inherently an inverse problem under *uncertainty*, which may arise at every stage of catalyst design, e.g., from noisy, incomplete observations to approximations in models. Current inverse optimization workflows struggle to represent and communicate uncertainty, especially as problem complexity grows. Uncertain visualization has the potential to enhance the inverse optimization problem by providing intuitive and practical tools to capture multiple sources of uncertainty. However, data's ever-increasing size and complexity pose fundamental challenges to existing visualization techniques. For example, combining ensemble simulations with surrogate models (common in large-scale DOE applications) introduces layered uncertainties that are hard to reconcile and present clearly. Users need to understand how uncertainties in data and model together affect the inverse solution, but existing tools often fail to clarify these complex relationships.

Opportunity: Effective uncertainty visualization bridges technical complexity and human insight, transforming uncertainty from a barrier into a strategic asset. Tailored tools can align with domain expertise, helping researchers prioritize robust designs and avoid unstable configurations. For example, integrating uncertainty visualization into catalytic digital twins (virtual models of reactors updated with operando data) could revolutionize high stakes catalyst testing. Domain scientists could assess not just predicted activity/selectivity/stability but also the confidence behind these metrics, adjusting reaction conditions to balance performance and catalyst deactivation risks. For the DOE, such tools translate raw error bounds into actionable insights, enabling bottom-up designs of catalyst architectures for impactful physical, chemical and biological transformations.

Uncertainty-aware visualization also offers a roadmap for accelerated catalyst discovery. From DOE facilities like light sources or supercomputers, visualizing uncertainties in inferred parameters (e.g., adsorption energies, surface coverage) can guide scientists to experiments that resolve critical ambiguity. Interactive dashboards can map how proposed spectroscopy experiments or atomic simulations decrease uncertainties in material properties, accelerating discovery with fewer trials. Similarly, in hybrid models blending physics and AI, visualization can flag regions where surrogate models extrapolate beyond reliable data (e.g., predicting alloy stability under extreme temperatures or pressures), guiding targeted operando data collection or high-fidelity simulations.

By embracing these approaches, DOE can overcome the needle-in-a-haystack search for optimal catalysts, accelerating breakthroughs in energy and critical materials.

Innovation: Realizing these opportunities demands breakthroughs in uncertainty-aware visual analytics and human-AI collaboration:

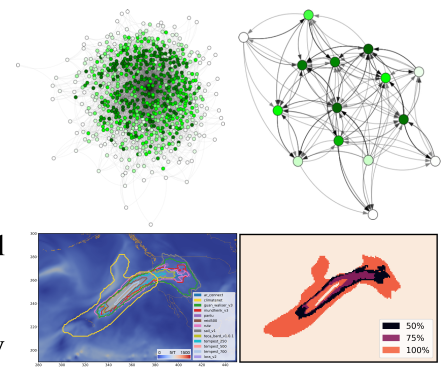

Figure 1: Top: Visual representation of chemical reaction spaces as a graph. Bottom: Atmospheric rivers and their uncertainty visualization.

1. High-Dimensional Uncertainty Visual Encoding: Develop intuitive tools to visualize uncertainty in high-dimensional parameter and solution space. Techniques involve data abstraction, structure extraction, and simplification to arrive at a compact and hierarchical representation (Figure 1, top) and quantifying and incorporating uncertainty information for visual exploration to reveal hidden solution modes (Figure 1, bottom).

2. Interactive Optimization Interfaces: Embed visualization directly into optimization loops. For example, real-time Pareto frontiers with uncertainty bands could let users adjust objective weightings (e.g., prioritizing stability over activity) while instantly seeing how risks shift. Integrated "proof sketches" might visually trace how data or model assumptions drive specific solutions, building trust in AI-generated designs.

3. Uncertainty-aware human-AI collaboration: Uncertain visualization also has the potential to integrate human feedback into machine learning models, where human involvement can build trust in the system and provide insights into its decision-making process. While AI can train generative models to learn the distribution of solutions, humans can annotate areas of concern and propagate those annotations back into the computational model (closing the loop between qualitative expert judgement and quantitative analysis).

In conclusion, making visualization uncertainty a cornerstone of optimization algorithms for inverse problems will enable users to fully exploit advances in computation and data. Investing in uncertainty-aware visualization research will lay the groundwork for inverse methods that are not just mathematically optimal, but also cognitively and practically optimal for human decision-makers. This alignment of computational and human perspectives will be key to tackling the next generation of scientific challenges under uncertainty.