GenMatLab: A Generative Platform for Inverse Materials Design

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Abstract

In this demo, we present GenMatLab, a user-friendly web platform that makes latest AI techniques accessible for inverse materials design. The platform integrates data analysis and generative modeling into an easy-to-use interface, enabling researchers, material domain experts, and practitioners to explore and apply AI techniques without requiring advanced coding expertise. At its core are generative AI models that support interactive operations, allowing users to conduct inverse design and investigate generated candidates in an intuitive and exploratory way. By lowering technical barriers, GenMatLab empowers a broader community to leverage cutting-edge AI methods for accelerating materials discovery.

Introduction

Inverse materials design has emerged as a critical task in accelerating the discovery of novel materials. Unlike traditional trial-and-error approaches, inverse design starts from desired material properties and working backwards to identify candidate structures that meet users' requirements. This paradigm is particularly valuable in domains such as energy storage, semiconductors, and aerospace, where efficient exploration of design spaces can save both time and resources (Han et al. 2025). With the growing availability of machine learning and generative models, inverse design has become increasingly data-driven, enabling researchers to move beyond heuristic-based methods and towards systematic, AI-assisted discovery (Wang et al. 2023).

Despite these advances, most AI-based approaches to inverse design remain difficult to access for non-expert users. Implementations are often fragmented across research codebases, requiring substantial programming expertise and computational resources to operate effectively. This creates a substantial barrier for material domain experts, practitioners, and others who wish to apply modern AI methods to their own problems. Several toolkits and infrastructures already play an important role in advancing materials research. The Materials Project serves as a powerful analysis platform, providing large-scale computational data and visualization tools for exploring material properties (Horton et al. 2025). The JARVIS infrastructure offers rich databases and associated tools that support computational materials science (Choudhary 2025). The Open MatSci ML Toolkit provides standardized benchmarks and workflows for machine learning in solid-state materials modeling (Miret et al. 2022). While these resources are invaluable for data access, analysis, and benchmarking, none of them directly support interactive inverse materials design workflows, highlighting the unique contribution of GenMatLab.

To the best of our knowledge, GenMatLab is the first platform that provides an integrated, user-friendly environment for inverse materials design. This website offers an accessible and interactive environment where users can conveniently conduct data analysis and generative tasks for inverse design. At its core, the platform leverages generative AI models to support interactive exploration, enabling users to design materials from target properties and investigate generated candidates in an intuitive manner. By lowering technical barriers, GenMatLab makes generative AI techniques usable "for all", thereby supporting a broader community.

Functionality of GenMatLab

User Interface As shown in Fig. 1, the GenMatLab interface is designed to be intuitive, modular, and user-friendly, ensuring that material domain experts and practitioners can conduct inverse design without requiring programming expertise. At the top of the interface, users are guided through a structured workflow with clearly labeled sections. This navigation panel provides a logical progression from dataset preparation to generative candidate exploration, making it straightforward to follow the entire design pipeline.

Inverse Design with Multiple Target Properties We demonstrate the user interaction page through the multi-target generation task. On the left hand side of the panel, users can specify material properties (e.g., Strength, TC1, EC2) as inverse design objectives. A model can be chosen as well (e.g., Tab-DDPM-Reg) and its corresponding adjustable parameters are provided. Then users can input desired target values for the selected properties, with both high-level interactive controls and underlying command-line code snippets displayed, ensuring reproducibility and accessibility for users with varying technical backgrounds.

To support interpretation, GenMatLab provides an interactive t-SNE visualization panel, which projects both origi-

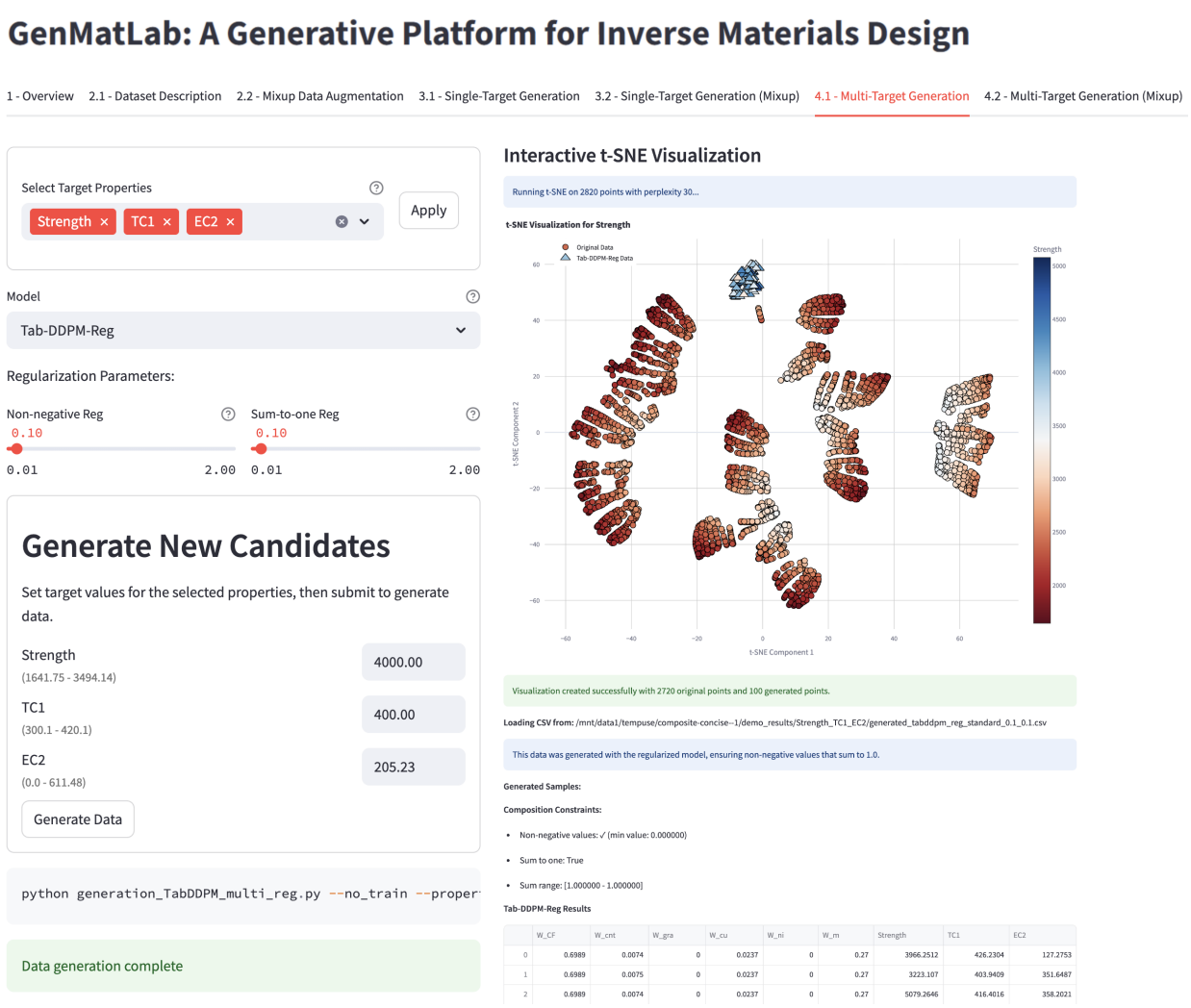

Figure 1: GenMatLab interface for multi-target inverse materials design.

nal and generated samples into a 2D space. This visualization allows users to compare the distribution of generated candidates against the dataset, observe patterns and evaluate how well generated data align with target specification. Meanwhile, the generated candidates are presented in the tabular form, allowing users to download the results. Together, these components create an integrated environment where users can seamlessly move from design goals to analyzing generated solutions in an interactive manner.

Backend Conditional Generative Model Training Inverse materials design requires generative models that can produce candidate structures conditioned on user-specified target properties. To support this need, we integrate conditional generative models including cVAEs (Harvey, Naderiparizi, and Wood 2021) and TabDDPM (Kotelnikov et al. 2023) to enable property-guided sampling in low- to medium-dimensional design spaces. In addition, GenMatLab adopts PCDiff (Qian et al. 2025), a latest diffusion-based generative model designed for tabular material data, which has demonstrated strong performance in generating high-quality candidates under property constraints.

Data Augmentation High-quality data is essential for effective inverse materials design, yet in practice, material datasets are often small, sparse, or imbalanced across property ranges. To address this challenge, GenMatLab includes a dedicated data augmentation method, i.e., Mixup (Zhang et al. 2017), to enable users to enrich datasets before generative modeling. By providing an intuitive interface for applying these techniques, GenMatLab empowers users to synthesize more representative datasets, ultimately enhancing the performance of downstream inverse design tasks.

Conclusion

In this technical demo, we introduce GenMatLab to serve as an easy-to-use platform for inverse materials design. Users can set target properties, generate candidates and explore results seamlessly. Overall, it serves as a practical tool that makes AI methods accessible for materials discovery.

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