# UniMate: A Unified Model for Mechanical Metamaterial Generation, Property Prediction, and Condition Confirmation


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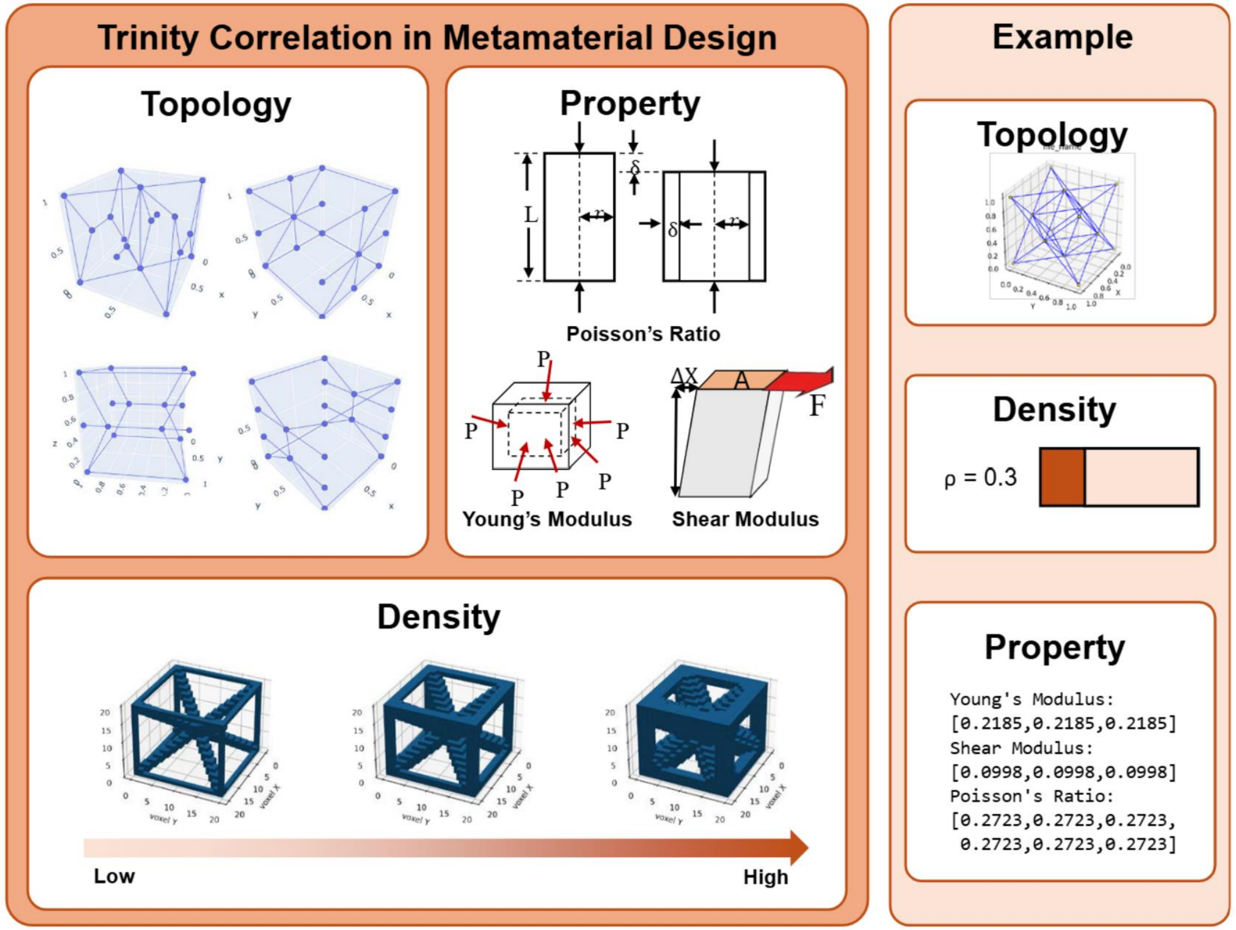
# Background – Mechanical Metamaterial Preliminary

- **Definition:** Artificially engineered materials whose properties arise from their internal structure rather than chemical composition.
- **Key Characteristics:**
  - **Programmability:** Internal structures can be designed to exhibit tailored responses.
  - **Tunability:** Properties such as stiffness, density, and wave propagation can be adjusted through structural design.
  - **Unconventional Behavior:** Capable of achieving properties not typically found in natural materials.
- **Applications:** Aerospace, biomedical implants, energy absorption systems, etc.

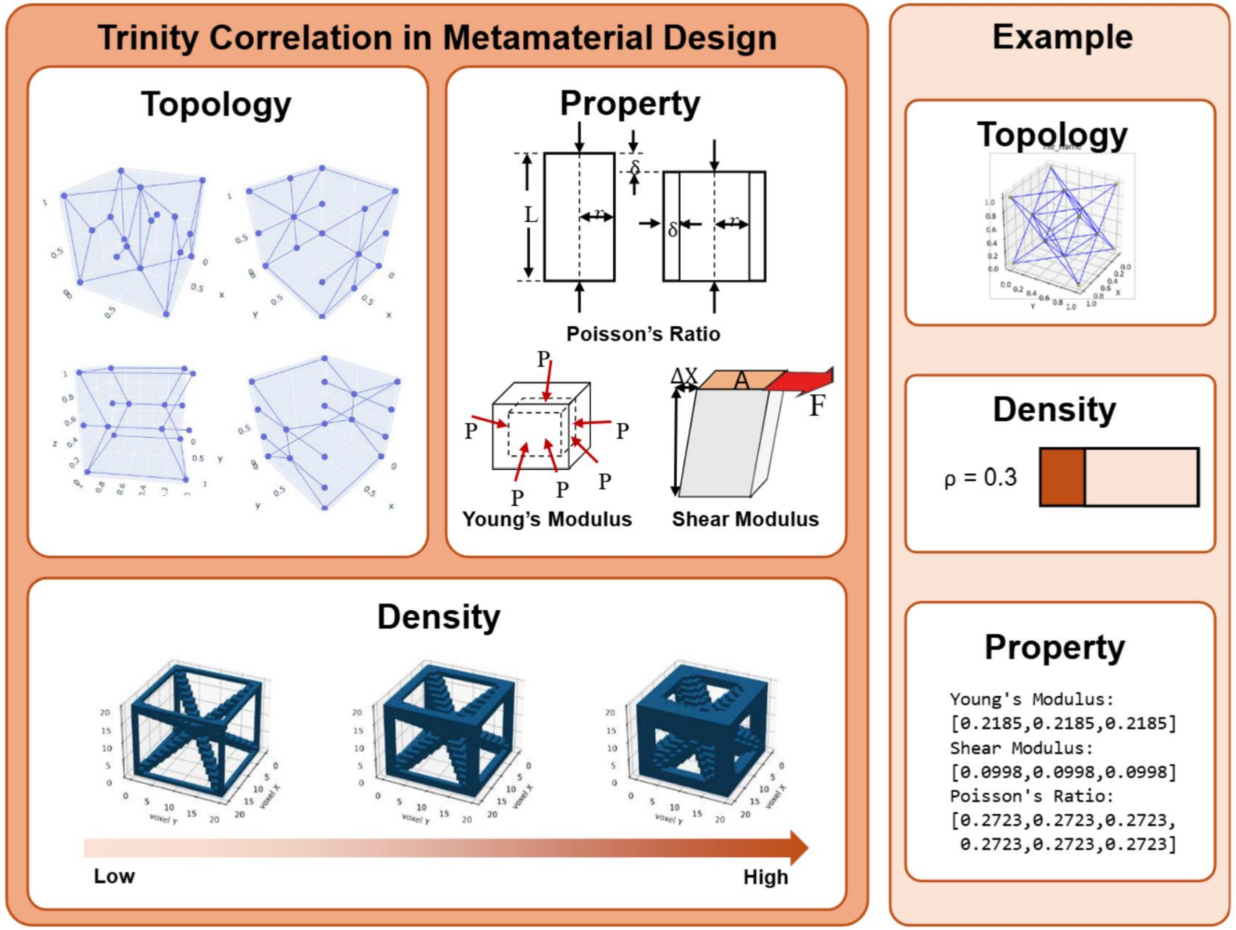


# Background – Challenges in Metamaterial Design

## ❑ Data Complexity:
- Three modalities: topology (3D graphs), density, and properties.

## ❑ Task Diversity:
- property prediction, topology generation, condition confirmation.

## ❑ Lack of Benchmarks:
- Existing models focus only on subsets of tasks; Inadequate datasets for comprehensive evaluation.



# Methodology – Framework Overview

❑ **Goal:**

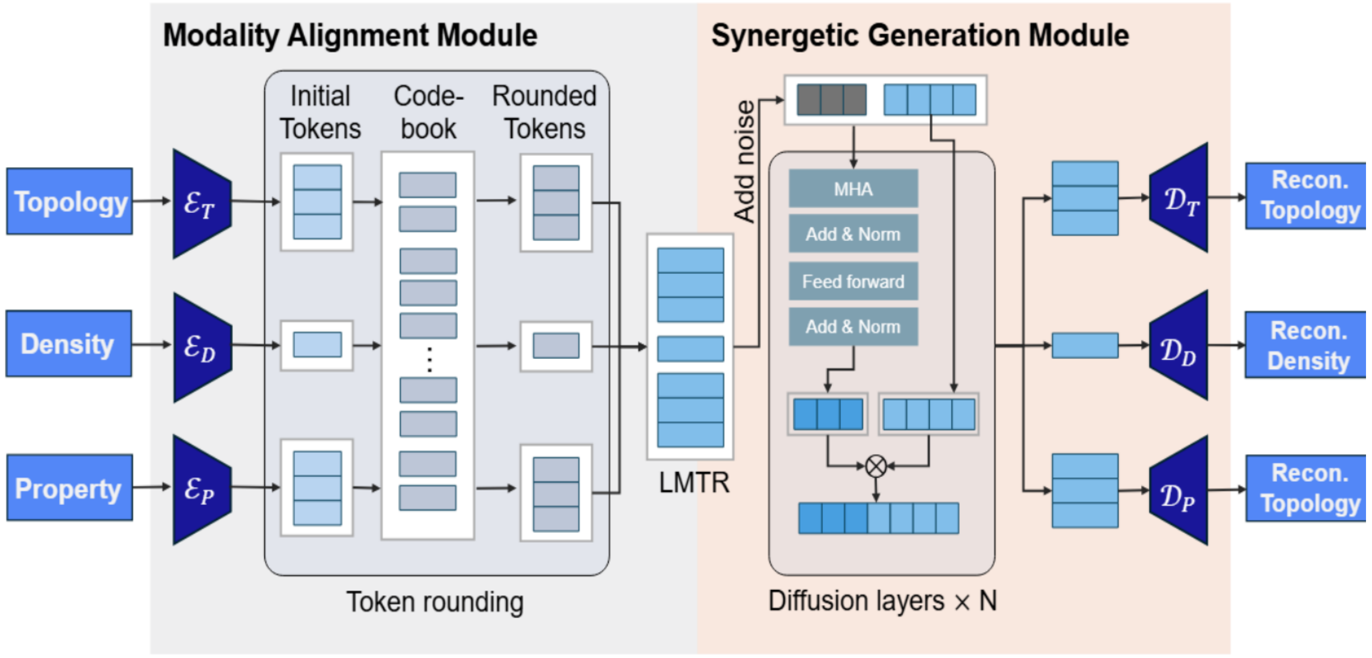
- Unified modeling of all metamaterial modalities and tasks.

❑ **Two Key Modules:**

- **Modality Alignment Module:** Compresses and aligns modalities.
- **Synergetic Generation Module:** Generates unknown modalities via guided diffusion.

❑ **Input/Output:**

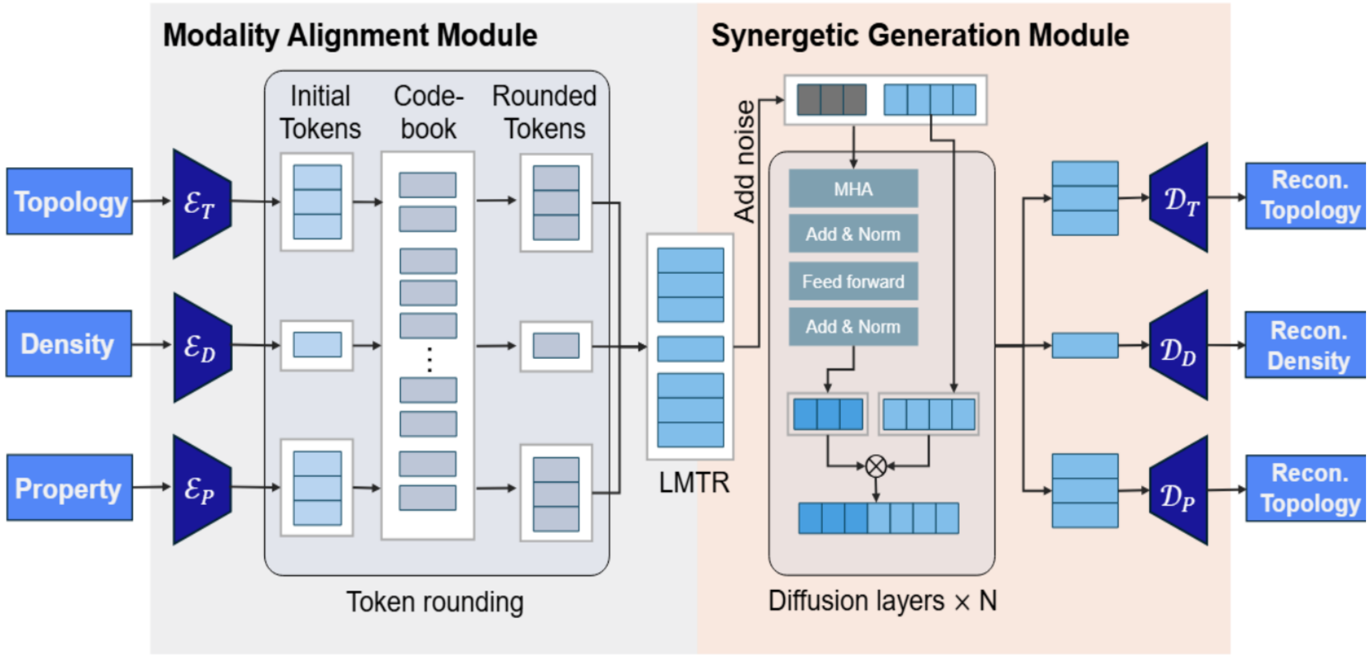
- Accepts any two modalities, completes the third.



# Methodology – Modality Alignment Module

❑ Aligning Diverse Modalities:

- **Step 1**: Encode each modality into discrete latent tokens.
- **Step 2**: Map all tokens into shared latent space.
- **Step 3**: Align using Tripartite Optimal Transport (TOT).




❑ **Benefit:**

- Establishes coherent joint representation across structure, condition, and property.

# Methodology – Synergetic Generation Module

## ❑Core Idea:

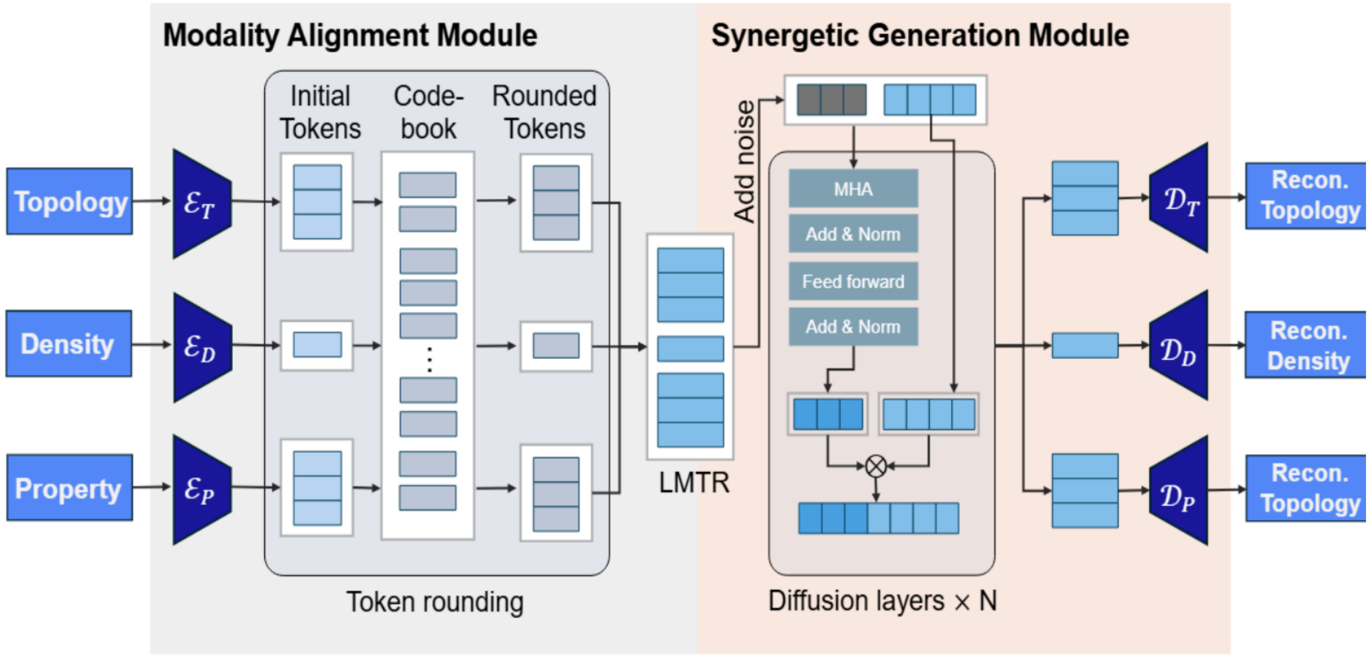
- Predict missing modality using known tokens as context.

## ❑**Method** (Partially Frozen Diffusion):

- Noise is added only to missing tokens
- Known tokens remain unchanged through transformer layers.

## ❑Why It Matters:

- Enhances robustness, task flexibility, and cross-modal generation.



# Results and Analysis – Performance Evaluation

## ❑ Evaluation Data & Metrics:

- **Dataset**: 15000 samples (material structure, properties and manufacturing condition), developed by our team.
- **F_qua:** structure generation quality.
- **F_cond:** condition matching error.
- **NRMSE_pp:** property prediction error.
- **NRMSE_cc:** condition confirmation error.

## ❑ Baseline Models:

- State-of-the-art material structure generation / property prediction models are included into the self-evaluation.

| Category | Models |
|---|---|
| **Generation-Only** | CDVAE, SyMat |
| **Prediction-Only** | Equiformer, ViSNet, MACE+VE |
| **Dual-Task (Prediction + Gen.)** | UniTruss |
| **UNIMATE (ours)** | Handles all 3 tasks in a unified framework |

## ❑ Results and Remarks:

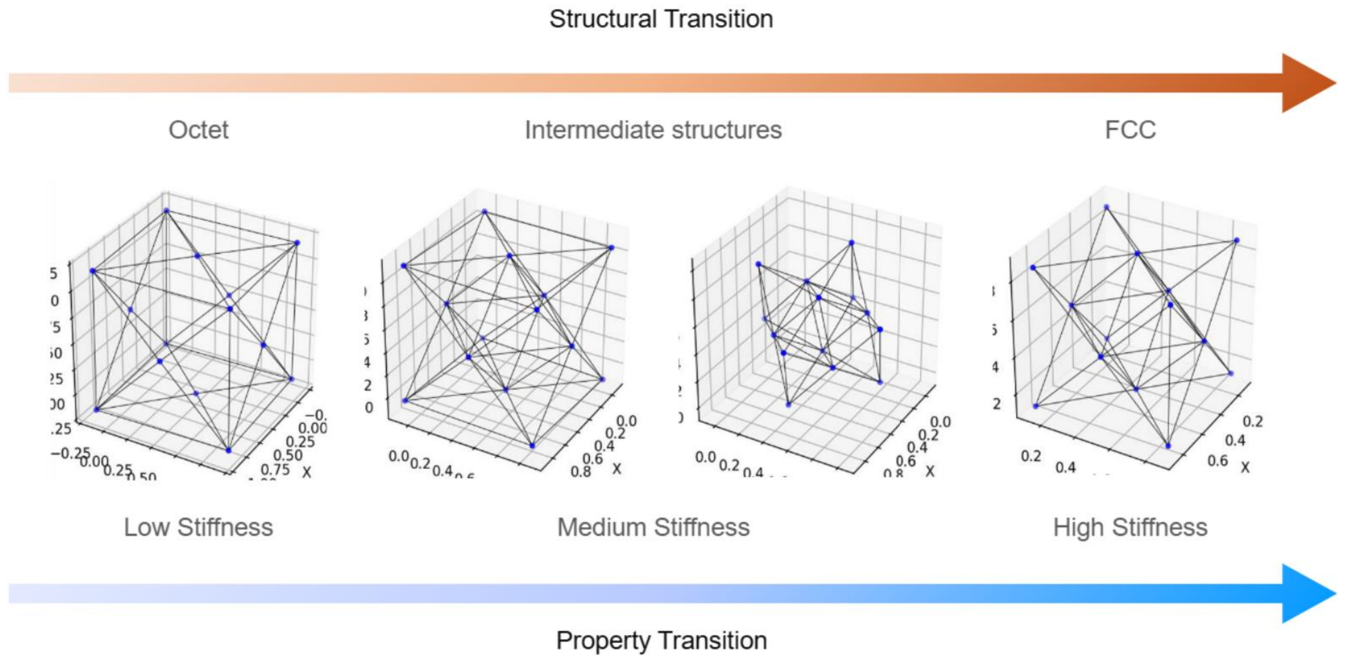
- UniMate compared with second best model: **80.2% less error** in generating material based on property, **5.1% less error** in predicting material properties, **50.2% less error** in confirming manufacturing condition.
- The strong **cross-modality alignment** of UniMate enables superior performance across diverse tasks.

*Table 2.* Effectiveness Comparison.

| Model | Topo. Gen. Task | | Prop. Pred. Task | Cond. Confirm. Task |
|---|---|---|---|---|
| | $F_{\text{qua}}$ ($\times 10^{-2}$, $\downarrow$) | $F_{\text{cond}}$ ($\times 10^{-2}$, $\downarrow$) | $\text{NRMSE}_{\text{pp}}$ ($\times 10^{-2}$, $\downarrow$) | $\text{NRMSE}_{\text{cc}}$ ($\times 10^{-2}$, $\downarrow$) |
| CDVAE (Xie et al., 2022) | 19.23 | 32.71 | N/A | N/A |
| Equiformer (Liao & Smidt, 2022) | N/A | N/A | 5.31 | 38.05 |
| ViSNet (Wang et al., 2024) | N/A | N/A | 3.12 | 10.43 |
| SyMat (Luo et al., 2024b) | 16.94 | 33.37 | N/A | N/A |
| UniTruss (Zheng et al., 2023a) | 19.43 | 33.77 | 2.71 | 8.89 |
| MACE+VE (Grega et al., 2024) | N/A | N/A | 2.57 | 9.09 |
| UniMate (Ours) | **2.74** | **7.81** | **2.44** | **4.43** |

# Results and Analysis – Case Study

- ❑ **Application Task:** Designing for light material with high stiffness.
- ❑ **Setup**: Fixed low density (e.g., 0.3), varied target stiffness.
- ❑ **Findings**: Model generates topology transitions from intermediate to known; Able to interpolate and propose **structures unseen by the model.**



# Conclusion

## ❑ Summary of Work:

- We proposed **UniMate**, a unified model that integrates multiple data modalities to support diverse tasks in mechanical metamaterial design.

## ❑ Key Contributions:

- Formulated metamaterial design as a multi-modal completion task.
- Proposed a unified model with modality alignment and synergetic diffusion.
- Built a benchmark dataset with standardized metrics.

## ❑ Impact of Work:

- Enables flexible and condition-aware inverse design.
- Advances data-driven methods for complex material systems.

Project Link: https://github.com/wzhan24/UniMate

# Thanks!

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