

## MIZOGUCHI LAB.

## Paving the way for Materials Design



Department of Materials and Environmental Science

Nano-Materials Design

Department of Materials Engineering, Graduate School of Engineering

<https://nmdl-mizo.github.io/en/>

## Our Mission: Paving the way for Materials Design

What kind of Structures?  
How to bring about the Properties?

Property ↔ Structure

Correlations and Mechanisms

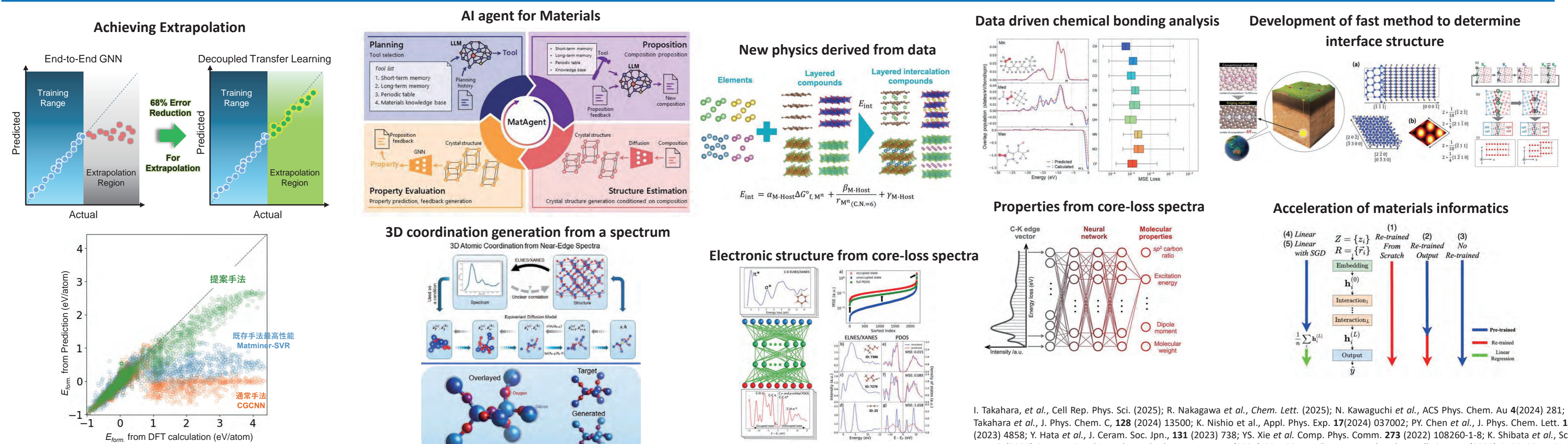


## Property-Structure Relationship for Materials Design

For decades, materials development has been driven by trial and error. That paradigm is now changing. Our vision is the realization of Designed Materials — a new frontier in which atomic arrangements are deliberately engineered to achieve target functionalities, bringing into existence structures that nature alone would never produce. At the heart of this vision lies a deep understanding of structure-property relationships — the connections between atomic and electronic structure and material function. By deciphering, at the level of chemical bonding, exactly where and how function emerges, we transform materials from something to be discovered into something to be designed.

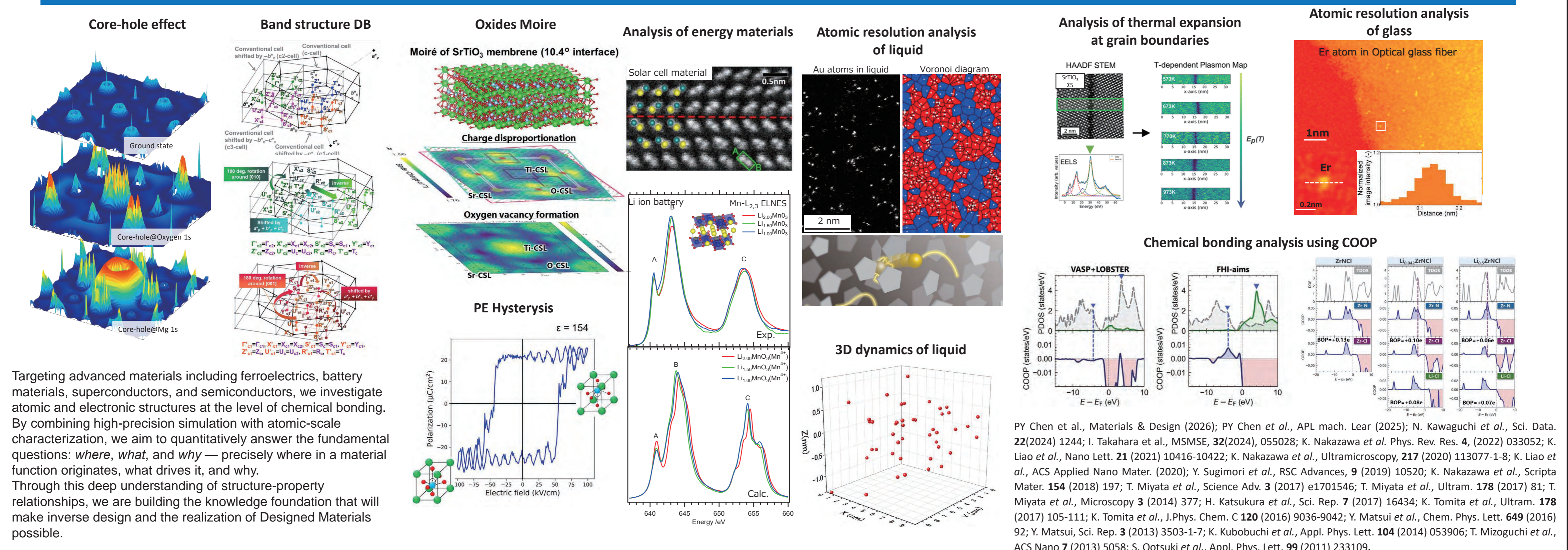
The Mizoguchi Laboratory integrates artificial intelligence, computational simulation, and atomic-scale characterization into a seamless research pipeline — driving the full cycle from the elucidation of structure-property relationships to the practical implementation of materials design.

## AI for Material



The Mizoguchi Laboratory advances research at the intersection of artificial intelligence — encompassing generative AI, large language models (LLMs), and AI agents — with computational simulation and atomic-scale characterization. Through inverse design, in which target functionalities drive the determination of atomic arrangements, we fundamentally reimagine materials exploration beyond conventional trial and error. Within an agentic cycle where AI autonomously generates and tests hypotheses, humans and AI collaborate to unravel structure-property relationships — propelling the transformation from a materials science that discovers to one that designs.

## Understanding role of atom and chemical bonding



Targeting advanced materials including ferroelectrics, battery materials, superconductors, and semiconductors, we investigate atomic and electronic structures at the level of chemical bonding. By combining high-precision simulation with atomic-scale characterization, we aim to quantitatively answer the fundamental questions: *where*, *what*, and *why* — precisely where in a material function originates, what drives it, and why. Through this deep understanding of structure-property relationships, we are building the knowledge foundation that will make inverse design and the realization of Designed Materials possible.

