T. Mizoguchi LAB.

[Understanding the Role of Atoms and Electrons]

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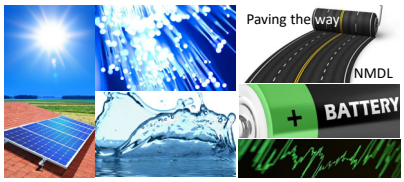
1 Materials Design ～Paving the Way for Materials Design～

What kind of Structures?
How to bring about the Properties

Property ⟷ Structure

Relationship

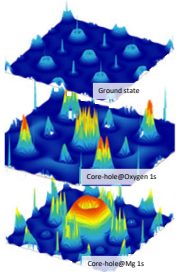


Property-Structure Relationship for Materials Design

Much higher performance and higher reliability are now required to the materials to achieve further technology developments. In case of electroceramics, such as multi-layer ceramic capacitor and varistor, the size of grains in devices becomes smaller and smaller, and further property improvements of each grain and grain boundary are desired. To achieve this, clarification of atomic and electronic structures and finding the way to improve their properties are indispensable.

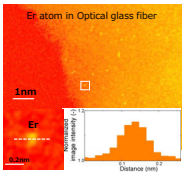
In our group, atomic and electronic structure are investigated by combining electron energy loss spectroscopy (EELS), transmission electron microscopy (TEM), first principles calculation. By combining these methods, atomic and electronic structures and their relationships with materials properties can be unraveled.
Particularly, superlattice, ionic liquid, Li-ion battery, photovoltaic cell, electroceramics, and glass are investigated.

2 Seeing Atoms & Bonding

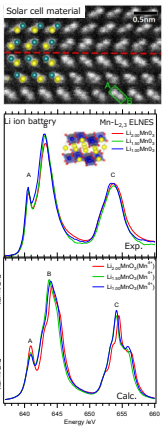


We are investigating electron-energy-loss near-edge structures (ELNES) and X-ray absorption near-edge structures (XANES) from experimental and theoretical viewpoints. ELNES and XANES originate from the electron transition from a core orbital to unoccupied bands. Their spectral features reflect the partial density of states of unoccupied bands, which contains information on the atomic and electronic structures.
Experimentally, spatial- and time- resolved ELNES can be obtained at high accuracy by STEM-EELS.
On the other hand, theoretical calculation is necessary to interpret the experimental spectrum. Including effect of core-hole, which is introduced by electron transition from core-orbital to conduction band, is indispensable to calculate spectrum structures correctly.

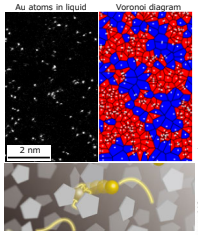
Atomic resolution analysis of glass



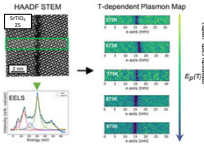
Analysis of energy materials

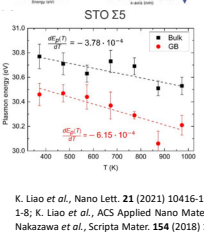


Atomic resolution analysis of liquid

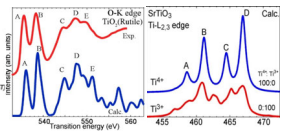


Analysis of thermal expansion at grain boundaries

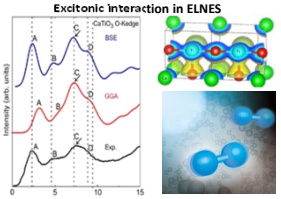




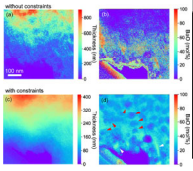
Single, Excitonic, Multiplet in ELNES



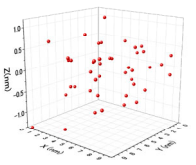
Excitonic interaction in ELNES



Analysis of glass phase separation



3D dynamics of liquid



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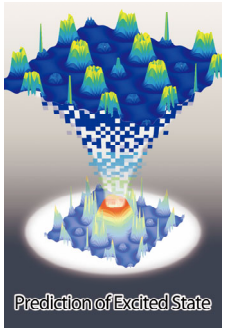
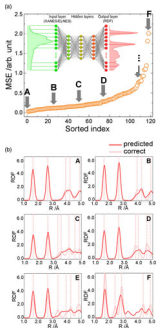
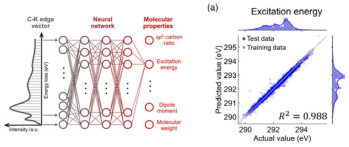
3 Understanding the Role of Atoms and Electrons in Materials

Data-driven prediction of structure from core-loss spectra

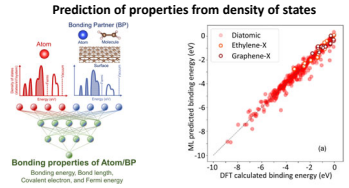




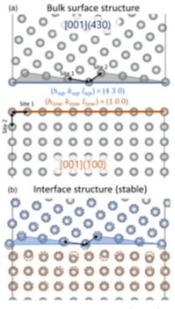
Prediction of properties from core-loss spectra



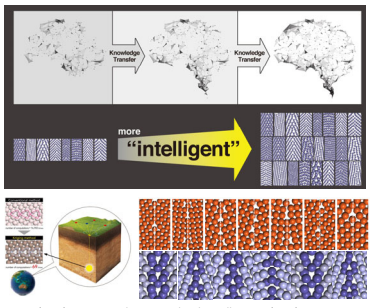
Prediction of properties from density of states



Direct prediction of gain boundary properties



Artificial Intelligence (AI) achieve 3,600 times higher efficiency



To design materials properties, we are investigating atomic and electronic structures quantitatively by performing high-precision simulations of atomic structures such as interfaces and lattice defects, which have a great impact on the functions of materials, and core excitation spectra, which show a variety of shapes reflecting electronic states. In addition, from the viewpoint of materials informatics, where information science is applied in materials research, we are applying machine learning methods such as transfer learning, Bayesian optimization, and virtual screening to interfaces, lattice defects, and inner-shell excitation spectra to understand and predict structure-function relationships.

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