Mizoguchi Research Group

[Understanding the Role of Atom and Electron]

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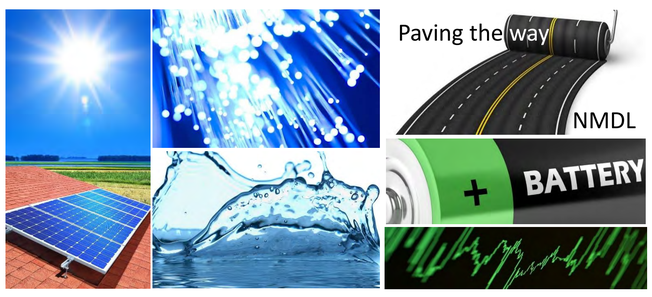
1 Materials Design ～Paving the Way for Materials Design～

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

Property ⟷ Structure

Relationship

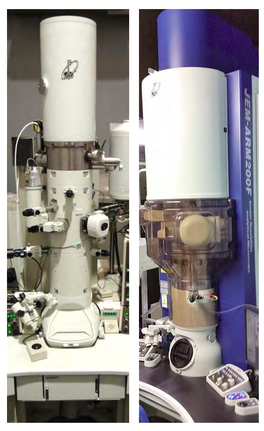


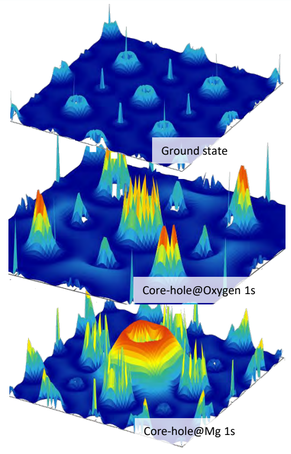
Property-Structure Relationship for Material Design

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.

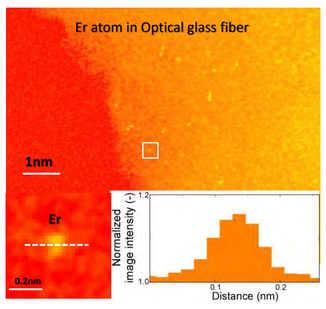
2 Seeing Atoms & Bonding



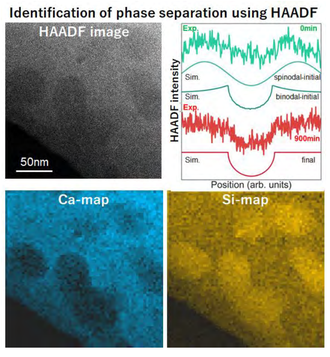


We are investigating electron-energy-loss near-edge structures (ELNES) and X-ray absorption near-edge structures (XANES) from experimental and theoretical viewpoints. ELNES and XANES originate from the electron transition from a core orbital to unoccupied bands. Their spectral features reflect the partial 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.

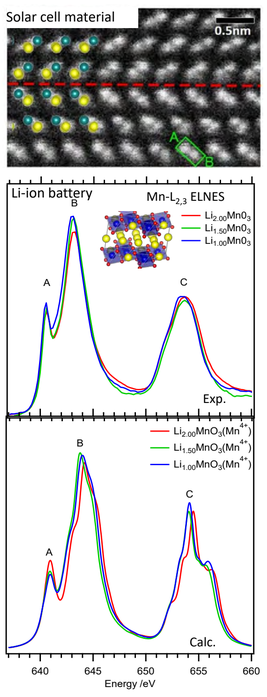
Atomic resolution analysis of Glass



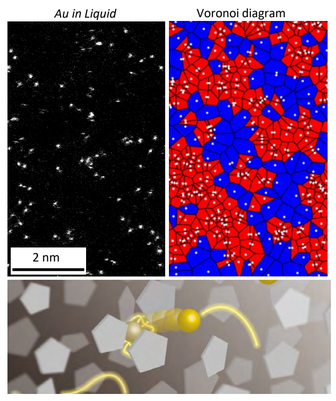
Identification of phase separation using HAADF



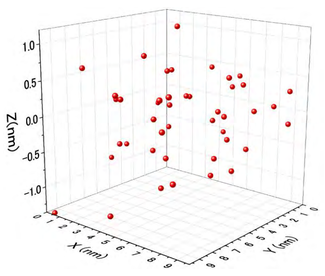
Analysis of energy materials



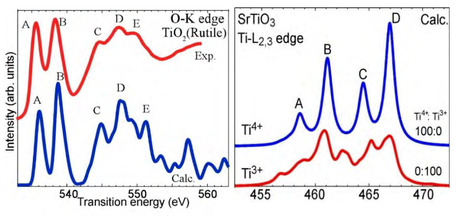
Atomic resolution analysis of Liquid



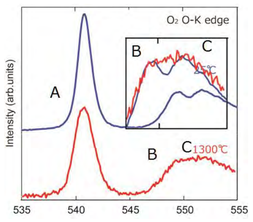
3D dynamics of liquid



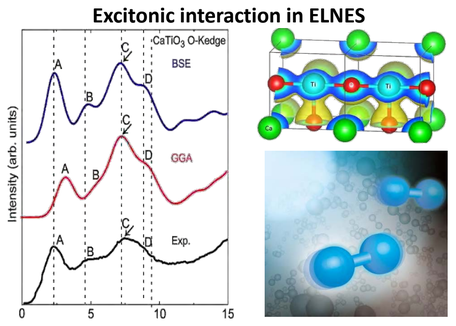
Single, Excitonic, Multiplet in ELNES

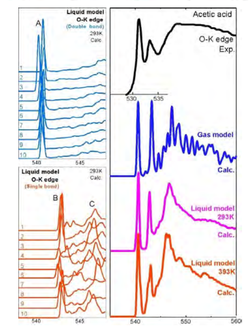


Liquid and Gas ELNES



Excitonic interaction in ELNES





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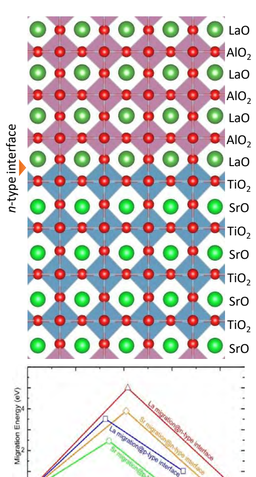
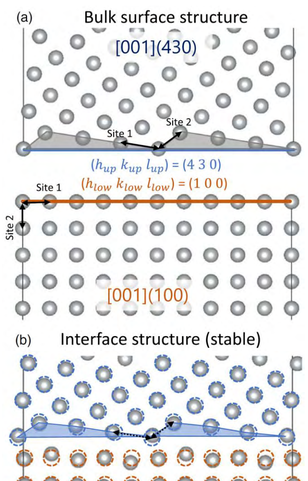
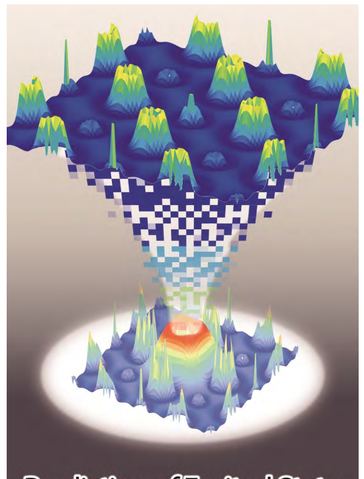
3 Understanding the Role of Atom and Electron in Materials

Understanding diffusion

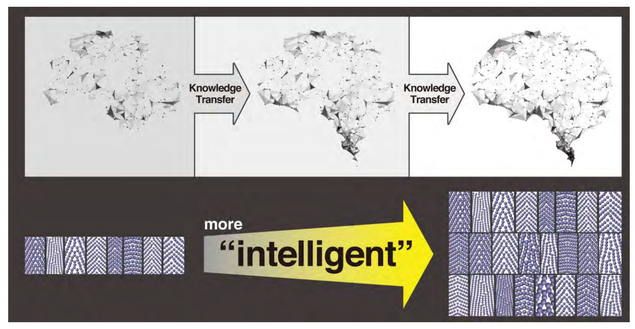


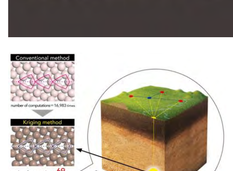
Acceleration of materials science using Machine Learning approach

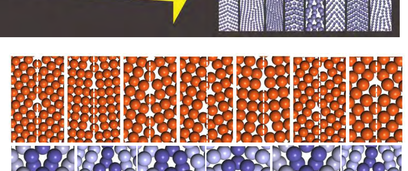




Artificial Intelligence (AI) achieve 3,600 times higher efficiency







Lattice imperfections such as vacancy, dopants, and grain boundary influence materials properties. To design materials properties, we investigate atomic and electronic structure of lattice imperfections, and attempt to pave the way for materials design with an aid of informatics approach.

Utilizing information science is an indispensable approach in materials science. We are applying informatics approach, such as transfer learning, Bayesian optimization, and virtual screening, to the interface, lattice imperfection, and spectrum. Using our machine-learning models, calculation cost for interface structure determination is significantly improved. We are also investigating property prediction from spectrum and interface configuration.

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