Mizoguchi Research Group

[Understanding the Role of Atom and Electron]

Institute of Industrial Science
Dept. Mater. Envi. Science

Nano-Materials Design Laboratory

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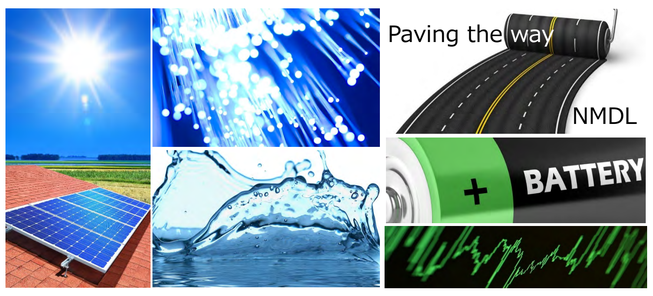
1 Materials Design ～Paving the Way for Materials Design～

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

Property ⟷ Structure

Relationship



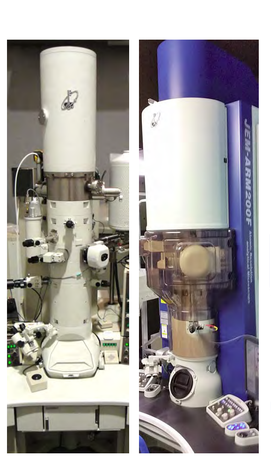
Research in Mizoguchi Research Group

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 their grains in electric devices becomes smaller and smaller, ca. 1mm or less, and thus 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 analysis of materials are investigating by combining electron energy loss spectroscopy (EELS), transmission electron microscopy (TEM), and first principles calculation. By combining those methods, atomic and electronic structures and their relationships to materials properties can be unraveled.

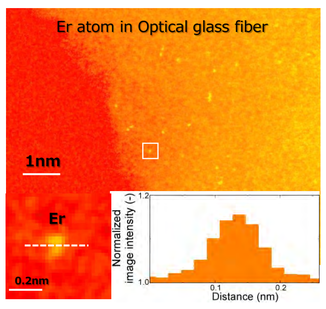
Particularly, superlattice, ionic liquid, Li-ion battery, Photovoltaic cell and electroceramics are investigated.

2 Seeing Atoms & Bonding

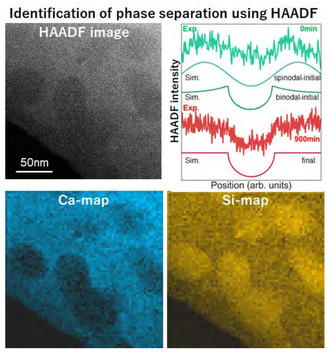


Since electron-energy-loss near-edge structures (ELNES) originate from the electron transition from a core orbital to unoccupied bands, spectral features of the ELNES reflect the partial density of states of unoccupied bands, and can provide information on the atomic and electronic structures. On the other hand, theoretical calculation of ELNES is necessary to interpret the spectrum. To calculate ELNES/XANES, core-hole, which is introduced in electron transition from core-orbital to conduction band, is indispensable. We are developing and applying theoretical ELNES/XANES.

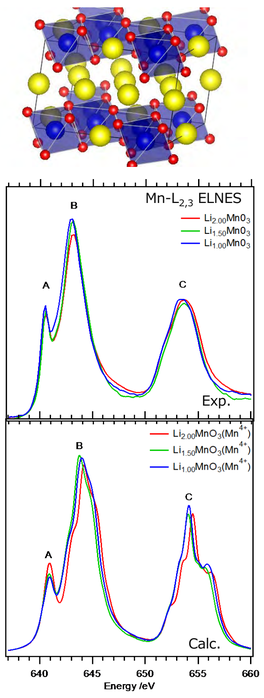
Atomic resolution analysis of Glass



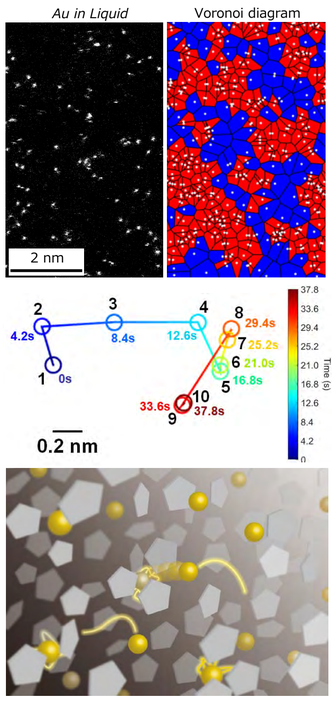
Identification of phase separation using HAADF



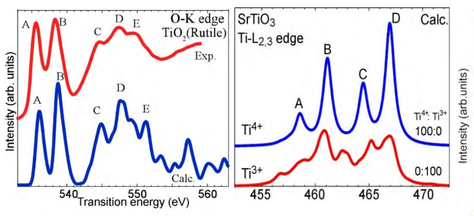
Li-ion battery



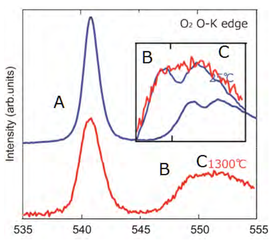
Atomic resolution analysis of Liquid



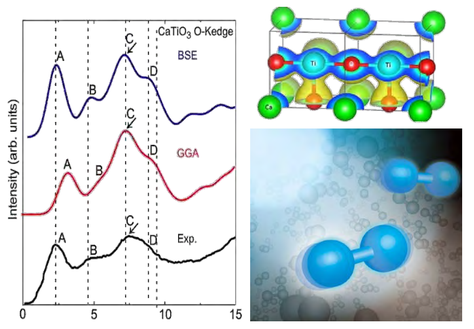
Single, Excitonic, Multiplet in ELNES

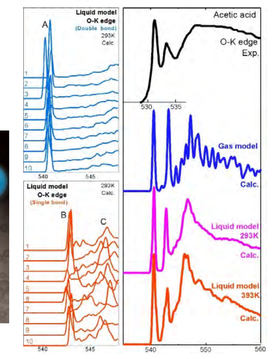


Liquid and Gas ELNES



Excitonic interaction in ELNES





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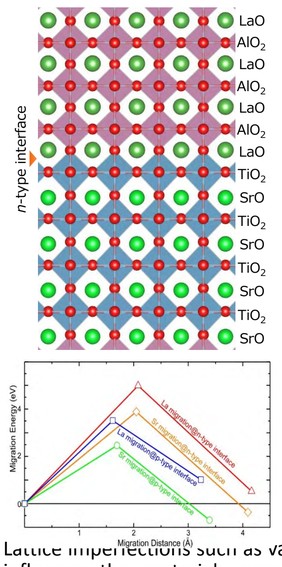
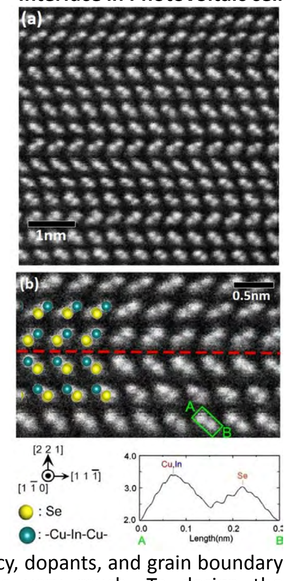
3 Understanding the Role of Atom and Electron in Materials

Understanding diffusion

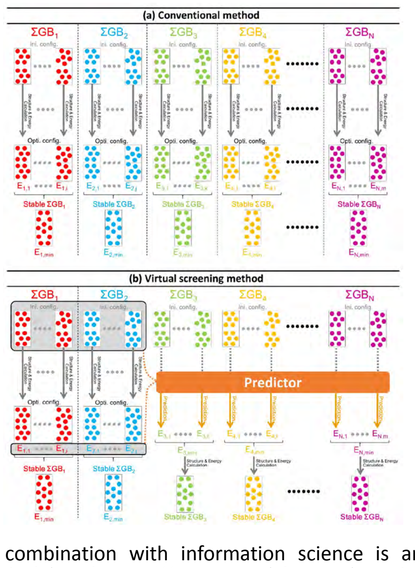


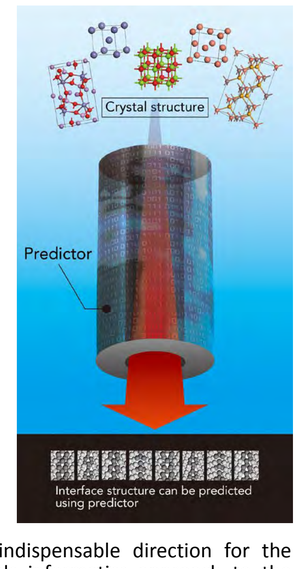
Interface in Photovoltaic cell



Lattice imperfections such as vacancy, dopants, and grain boundary influence the materials properties very much. To design the materials property, we investigate the atomic and electronic structure of those lattice imperfections, and attempt to pave the way for Materials Design with an aid of "Informatics" approach.

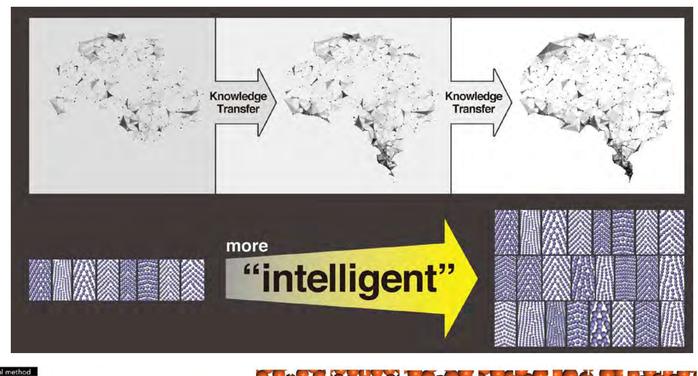
Acceleration of materials science using Machine Learning approach

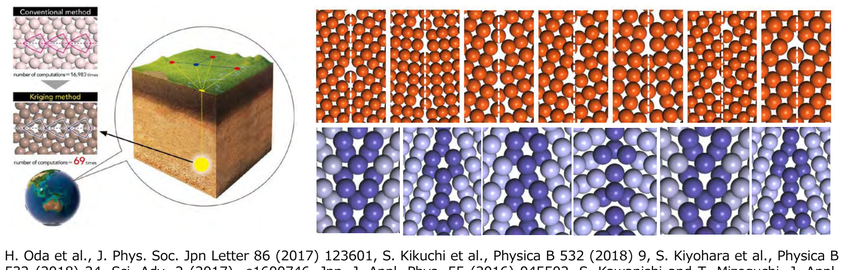




A combination with information science is an indispensable direction for the materials science. We are applying such materials informatics approach to the interface. Using our method, the speed for the structure determination of the interface is significantly improved. Furthermore, new findings were also discovered by our method.

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





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