

# Mizoguchi Lab.

## Institute of Industrial Science, Dept. Mater. Envi. Science

## Nano-Materials Design Lab.

http://www.edge.iis.u-tokyo.ac.jp

#### Materials Design $\sim$ Paving the way for Materials Design $\sim$

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

Property Structure

Paving the wa

BATTERY

Relationships

### **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.

## Atomic scale investigation using "The Ultimate Analysis"



electron-energy-loss near-edge structures originate from the electron transition from a core orbital to upied 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 applying theoretical ELNES/XANES.





ELNES calculation

Liquid ELNES

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## Materials Design using Lattice Imperfection Informatics



Institute of Industrial Science

Informatics on lattice imperfection in Photovoltaic cell

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