Mizoguchi Research Group

~Understanding role of atom and electron in material~

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

Nano-Materials Design Lab.

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

Materials Design　～Paving the way for Materials Design～

What's kind of Structures?
How to bring about the Properties
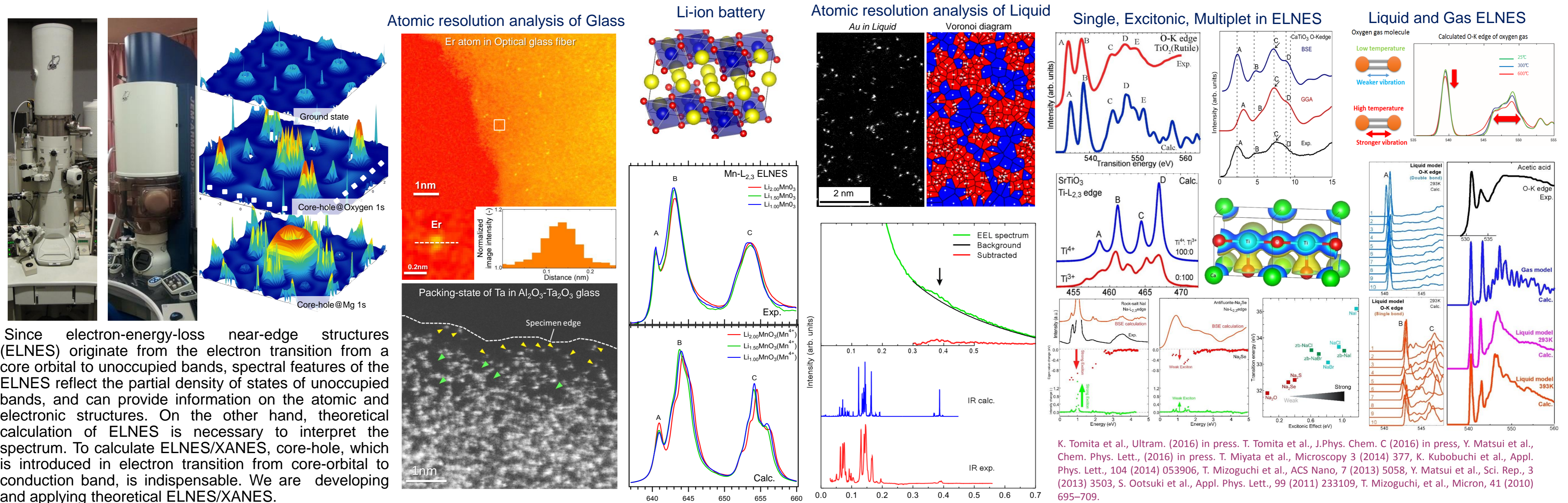
Property ⟷ Structure
Relationship

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.
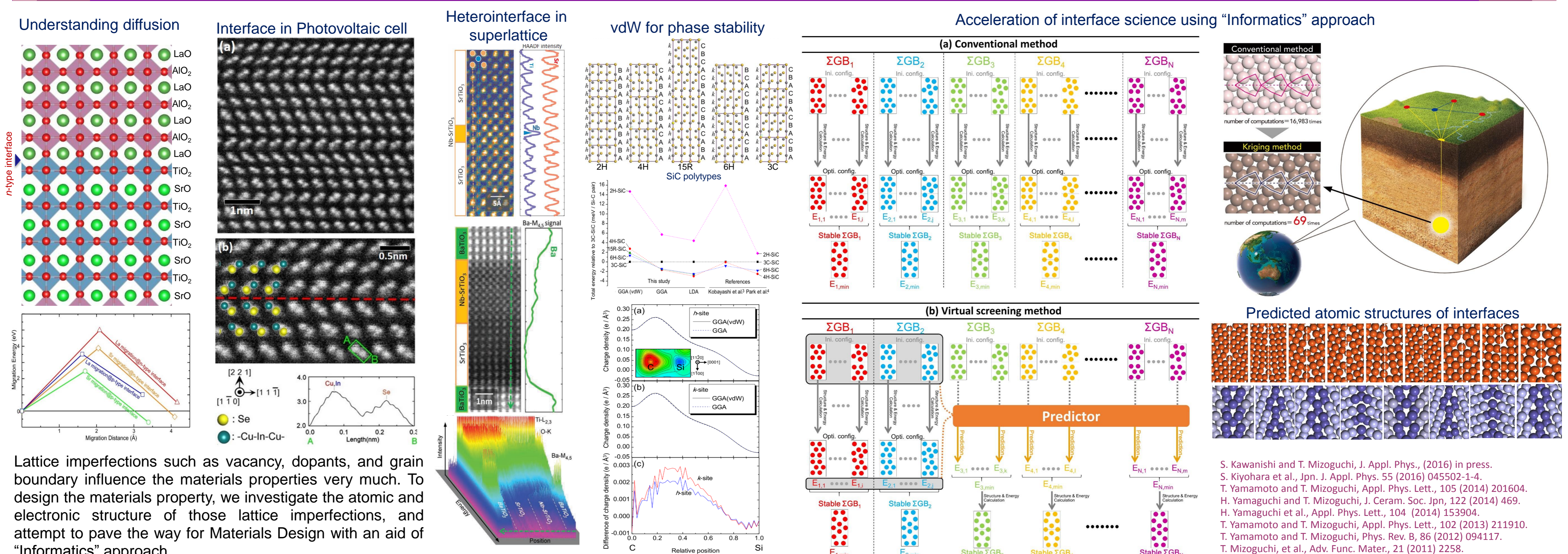
In our group, atomic and electronic structure analysis of materials are investigating by combining electron energy loss spectroscopy (EELS), transmission electron microscopy (TEM), and first principles calculation. By combining those methods, atomic and electronic structures and their relationships to materials properties can be unraveled.

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

Atomic scale investigation using "The Ultimate Analysis"

Atomic resolution analysis of Glass — Er atom in Optical glass fiber

Li-ion battery

Atomic resolution analysis of Liquid — Au in Liquid / Voronoi diagram

Single, Excitonic, Multiplet in ELNES

Liquid and Gas ELNES

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.

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Materials Design using Lattice Imperfection Informatics

Understanding diffusion

Interface in Photovoltaic cell

Heterointerface in superlattice

vdW for phase stability

Acceleration of interface science using "Informatics" approach — (a) Conventional method — (b) Virtual screening method

Predicted atomic structures of interfaces

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.

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