

# T. Mizoguchi LAB.

## [Understanding the Role of Atoms and Electrons]



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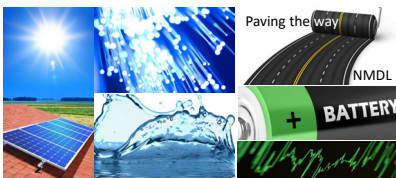
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### 1 Materials Design

~Paving the Way for Materials Design~

What kind of Structures?  
How to bring about the Properties



### Property-Structure Relationship 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**

**Analysis of glass phase separation**

**Atomic resolution analysis of liquid**

**Analysis of thermal expansion at grain boundaries**

**Single, Excitonic, Multiplet in ELNES**

**Excitonic Interaction in ELNES**

K. Liao et al., Nano Lett. **21** (2021) 10416-10422; K. Nakazawa et al., Ultramicroscopy, **217** (2020) 113077-113081; K. Liao et al., ACS Applied Nano Mater. (2020); Y. Sugimori et al., RSC Advances, **9** (2019) 10520; K. Nakazawa et al., Scripta Mater. **154** (2018) 197; T. Miyata et al., Science Adv. **3** (2017) e1701546; T. Miyata et al., Ultram. **178** (2017) 81; T. Miyata et al., Microscopy **3** (2014) 377; H. Katsukura et al., Sci. Rep. **7** (2017) 16434; K. Tomita et al., Ultram. **178** (2017) 105-111; K. Tomita et al., J. Phys. Chem. **120** (2016) 9036-9042; Y. Matsui et al., Chem. Phys. Lett. **649** (2016) 92; Y. Matsui, Sci. Rep. **3** (2013) 3503-17; K. Kubouchi et al., Appl. Phys. Lett. **104** (2014) 053906; T. Mizoguchi et al., ACS Nano **7** (2013) 5058; S. Ootsuki et al., Appl. Phys. Lett. **99** (2011) 233109.

### 3 Understanding the Role of Atoms and Electrons in Materials

**Data-driven prediction of structure from core-loss spectra**

**Prediction of Excited State**

**Prediction of properties from core-loss spectra**

**Prediction of properties from density of states**

**Direct prediction of grain boundary properties**

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

E. Suzuki et al. Appl. Phys. Express **14** (2021) 085503; K. Kikumasa et al., Adv. Intell. Syst., **4** (2022) 2100103-1-10; S. Kiyohara et al., Appl. Phys. Express **13** (2020) 065504; S. Kiyohara et al., npj Comp. Mater. **6** (2020) 68; R. Otani et al., Appl. Phys. Express **13** (2020) 065504; S. Kiyohara et al., J. Phys. Mater. **2** (2019) 024003; M. Tsubaki et al., J. Phys. Chem. Lett. **9** (2018) 5733; S. Kiyohara et al., Sci. Rep. **8** (2018) 13548; S. Kiyohara et al., J. Chem. Phys. **148** (2018) 241741; H. Oda et al., J. Phys. Soc. Jpn **86** (2017) 123501; S. Kiyochi et al., Physica B **532** (2018) 9; S. Kiyohara et al., Physica B **532** (2018) 24; S. Kiyohara et al., Sci. Adv. **2** (2017) e1600746; S. Kiyohara et al., Jpn. J. Appl. Phys. **55** (2016) 045502-1-4; S. Kawashiri and T. Mizoguchi, J. Appl. Phys. **119** (2016) 175101; T. Yamamoto et al., Appl. Phys. Lett. **105** (2014) 201604; H. Yamaguchi et al., J. Ceram. Soc. Jpn. **122** (2014) 469; H. Yamaguchi et al., Appl. Phys. Lett. **104** (2014) 153904; T. Yamamoto et al., Appl. Phys. Lett. **102** (2013) 211910; T. Yamamoto et al., Phys. Rev. B **86** (2012) 094117; T. Mizoguchi et al., Adv. Func. Mater. **21** (2011) 2258.