第 74回フロンティア材料研究所講演会

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8月16日（木） 13時30分～15時　R3棟1階会議室にて
演題：**The Enabling Roles of Hydrothermal Chemistry and Multiple Anions Leading to Noncentrosymmetry**

Multiple or mixed-anion compounds play a key design role in the discovery of novel noncentrosymmetric materials with large second-order dielectric responses ($\chi(2)$) that lack an inversion center. SHG-active crystals efficiently achieve frequency conversion to double the frequency of laser light to higher energies. One such material is the oxide-fluoride $KBe_2BO_3F_2$, or KBBF. SHG-active crystals often have anions with aligned polar moments in the solid state. Therefore, to synthesize highly-efficient SHG crystals, a promising strategy is to use the ***polarity*** of the d^0 early transition metal cations when they undergo out-of-center distortions (polar distortions) owing to electronic effects, specifically Second-Order Jahn-Teller distortions, and are displaced towards the oxide ligand(s) and the corner, edge, or face(s) of the anionic octahedra. The use of mixed–anions (oxide-fluorides) enhances the distortion of the anion as the metal-fluoride bonds contain less valence and thus creates stronger M=O bonds. ***Chirality*** is also an important concept in chemistry. Racemates are generally optically inactive due to the cancelation of opposite optical rotations from left- and right-handed enantiomers (*racemates*). However, specific arrangements of racemic units in the solid state can lead to optical activity and as many as one in twenty racemic compounds are potential optically active materials. For example, when considering the 21-noncentrosymmetric crystal classes, optical activity can be described as expected for not only pure isomers in the eleven-noncentrosymmetric enantiomorphic (chiral) point-groups, but also for racemates in four non-enantiomorphic point-groups.

References

H. Kageyama, K. Hayashi, K. Maeda, J.P. Attfield, Z. Hiroi, J.M. Rondinelli, K.R. Poeppelmeier, *Expanding frontiers in materials chemistry and physics with multiple anions*, **9**, 772 (2018).

連絡先：東　研究室（5315）