第 312　回応用セラミックス研究所講演会

講師：Professor K. R. Poeppelmeier
Department of Chemistry, Northwestern University

2月2日（火）　14時～16時　すずかけホール集会室1にて

演題：**Reimagine the Possible: Accelerating Materials Discovery**

The integrated process of predicting the functionality and stability of unreported compounds followed by laboratory synthesis and characterization has been successfully demonstrated for the 8 and 18-valence electron ABX family. Among the predicted and characterized properties of the missing ABX compounds are potential thermoelectric materials, topological semimetals, and transparent conductors (TCs).[1] This methodology could be expanded to more complex systems, such as the anion-deficient, fluorite structures that are particularly prominent in transparent conductors (TCs). The anion deficiencies produce many complex cation topological networks with varied local structures whose impact on TC properties is not understood. Indeed, thus far, only 6-coordinate cation sites have received any widespread attention in the TC field. $Ga_{3-x}In_{5+x}Sn_2O_{16}$ ($0.3 \leq x \leq 1.6$), or GITO, which has its own complex local structure which spans four differently coordinated sites.[2-5] Numerous other fluorite related materials are known. To gain a deep understanding of the optimal experimental conditions for synthesis, *in situ* neutron and X-ray diffraction studies are needed to proceed on a scale sufficient to investigate the large numbers of possibilities.

[1] Gautier, R.; Zhang, X.; Hu, L.; Yu, L.; Lin, Y.; Sunde, T.O.L.; Chon, D.; Poeppelmeier, K.R.; Zunger, A. *Nature*, **2015**, *7*, 308-316.
[2] Dolgonos, A.; Lam, K.; Poeppelmeier, K.R.; Freeman, A.J.; Mason, T.O. *J. Appl. Phys.*, **2014**, *115*, 013703.
[3] Dolgonos, A.; Wells, S.; Poeppelmeier, K.R.; Mason, T.O. *J. Am. Ceram. Soc.*, **2015**, *98*, 669-674.
[4] Rickert, K.; Sedefoglu, N.; Malo, S.; Caignaert, V.; Kavak, H.; Poeppelmeier, K. R. *Chem. Mater.* **2015**, *27*, 5072-5079.
[5] Rickert, K.; Huq, A.; Lapidus, S. H.; Wustrow, A.; Ellis, D. E.; Poeppelmeier, K. R. *Chem. Mater.* **2015**, 27, 8084-8093.

連絡先：東　研究室（5315）