

# 第111回フロンティア材料研究所講演会

講師: Professor James Neilson

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10月25日(金曜) 16時~17時30分  
大学会館2F 集会室1にて

## 演題: Enabling Prescriptive Synthesis of Metastable Ternary Oxides with Mixed Anions

Complex oxides enable a diverse set of electronic properties. However, we do not yet know how to prescriptively synthesize desired compositions or polymorphs of materials, particularly if they are metastable. Metathesis (or double-exchange) reactions are well suited to address synthesis questions pertaining to atomic transport and permit the identification of incipient stages of phase differentiation in solid-state reactions. As an example, the reaction,  $A_2CO_3 + Mn_2O_3 + YCl_3$ , where  $A = Li, Na, \text{ or } K$ , yields different Y-Mn-O products (and polymorphs) depending on which spectating alkali is present. From a combination of in situ and ex situ analysis of myriad synthesis reactions combined with first-principles calculation of thermodynamic parameters, we identify competent intermediates that enable kinetic control of the reaction, such as the phases  $LiMnO_2$  and  $YOCl$ . These results allow us to establish the critical processes in solid-state reaction pathways that enable, or hinder, prescriptive synthesis.



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