

## Cation and Anion Ordering in Complex Perovskites

*Patrick M. Woodward  
Department of Chemistry  
Ohio State University*

In this talk, I will discuss our studies of complex perovskites with a particular emphasis on atomic ordering over various length scales and its impact on the structure and properties of these materials. I'll begin by considering cation ordering of the smaller *B*-site cations. I will show some examples of perovskites where cation ordering is critical for properties and applications, and go on to discuss how order-disorder effects impact the powder diffraction patterns of these phases. Next, I will discuss two different examples of perovskites which undergo simultaneous ordering of the larger *A*-site cations and the smaller *B*-site cations. Using predictive design tools and high-pressure, high-temperature synthesis, a series of new  $\text{CaCu}_3\text{M}_2\text{M}'_2\text{O}_{12}$  ( $\text{M} = \text{Ga}, \text{Cr}$ ;  $\text{M}' = \text{Nb}, \text{Ta}, \text{Ru}$ ) phases have been prepared and characterized. The properties are shown to be very sensitive to the electronic interactions between  $\text{Cu}^{2+}$ ,  $\text{M}^{3+}$  and  $\text{M}'^{5+}$  ions. We have also been exploring  $\text{ALnMM}'\text{O}_6$  ( $\text{A} = \text{Li}^+, \text{Na}^+, \text{K}^+$ ,  $\text{Ln} = \text{rare-earth cation}$ ) perovskites where strong coupling between *A*-site ordering, *B*-site ordering and second order Jahn-Teller distortions of the *B*-site cations are all closely linked. Finally, if time permits, I will discuss our studies of oxynitride perovskites,  $\text{AMO}_2\text{N}$  ( $\text{A} = \text{Ba}, \text{Sr}, \text{Ca}$ ;  $\text{M} = \text{Ta}, \text{Nb}$ ), where novel dielectric behavior is closely linked to the details of the short range anion order.