Cation and Anion Ordering in Complex Perovskites

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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 CaCu₃M₂M′₂O₁₂ (M = Ga, Cr; M′ = Nb, Ta, Ru) phases have been prepared and characterized. The properties are shown to be very sensitive to the electronic interactions between Cu²⁺, M³⁺ and M′⁵⁺ ions. We have also been exploring ALnMM′O₆ (A = Li⁺, Na⁺, K⁺, Ln = 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, AMO₂N (A = Ba, Sr, Ca; M = Ta, Nb), where novel dielectric behavior is closely linked to the details of the short range anion order.