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# MSE 690 SEMINAR SERIES

## MONDAY, FEBRUARY 27TH | 3:45PM SEMINAR

## ARMS 1010


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## *"Interplay between structure, magnetism, and correlations in molybdate and nickelate perovskite oxides"*


**Abstract**: Perovskite oxides, with the ABO3 chemical formula, are the archetypical "quantum" materials, i.e., exhibiting an interplay between structural transitions, magnetic ordering, and electronic correlations, all occurring at similar energy scales. I will discuss two such examples where first-principles methods can be used to elucidate this interplay. First, I will discuss the case of rare-earth nickelates, which host a combined structural and metal-insulator transition with temperature, as well as the formation of long-range magnetic order. The nature of the complex antiferromagnetic (AFM) state in these materials is under debate experimentally, and often is not correctly reproduced with density-functional theory plus Hubbard U (DFT+U) calculations. By constructing ab-initio spin models via the local force theorem approach, we demonstrate the mechanisms for the formation of the AFM order, and the reasons for the experiment-theory discrepancy. The second example is that of molybdate perovskites such as SrMoO3, which has attracted attention for its record low room-temperature resistivity among perovskite oxides. Even though this material is considered weakly to moderately correlated, we show in this case via DFT plus dynamical mean-field theory (DMFT) calculations, that correct treatment of the Coulomb interactions and paramagnetism is crucial for accurate structural and spectral properties.


**Biography**: Cyrus Dreyer earned a B.S. in Engineering Science and Physics, and a B.A. in Mathematics from the University of Virginia. He earned a Ph.D. in Materials from the University of California, Santa Barbara, and then was a postdoctoral associate at Rutgers University. He is now an affiliate associate research scientist at the Flatiron Institute Center for Computational Quantum Physics, and an assistant professor at Stony Brook University in the department of Physics and Astronomy. His research interests involve developing and implementing computational techniques based on density functional theory to explore the properties of electronic materials.

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