

CHEMICAL ENGINEERING

SEMINAR SERIES



JAMES RONDINELLI

Monday, February 12, 2018

Associate Professor

Department of Materials Science and Engineering

Northwestern University

Learning from Data to Design Functional Oxides without Inversion

ABSTRACT: Accelerating the search for functional materials is a challenging problem. Here I describe an informatics-guided ab initio approach for accelerated design and discovery of noncentrosymmetric (NCS) crystals that find use in ferroelectric, piezoelectric, and nonlinear optical technologies. The workflow integrates group theory, data science methods, and quantum-mechanical calculations to uncover design guidelines for predicting NCS compounds. The key outcome is the identification of 242 compositions after screening ~3,200 that show potential for NCS structures, a 25-fold increase in the projected number of currently known Ruddlesden-Popper oxides without inversion symmetry. The data-driven predictions are assessed for 19 compounds using quantum mechanical calculations, among which 17 materials are found to be stable, including two potential multiferroics. Last, I discuss opportunities for combining data-science approaches into engineering curriculum, arguing that data-science methods are a fourth branch in materials science (alongside theory, simulation, and experimentation).

RECEPTION 3:30 • LECTURE 4:00 - 5:00
PHYSICS ASTRONOMY BLDG. PAA A 114



CHEMICAL ENGINEERING

UNIVERSITY of WASHINGTON

Knowledge and solutions for a changing world

BIOGRAPHY: James Rondinelli is the Morris E. Fine Junior Professor in Materials and Manufacturing at Northwestern University in the Materials Science and Engineering (MSE) Department, where he leads the Materials Theory and Design Group. His interests are in electronic structure theory and first-principles design of functional inorganic materials using picoscale structure-property relationships. In 2017, he was named the Materials Research Society (MRS) Outstanding Young Investigator. In 2016, he received a Sloan Research Fellowship in Physics, the Presidential Early Career Award for Scientists and Engineers (PECASE), and the 3M Non-Tenured Faculty Award. Additional honors include a NSF-CAREER Award (2015), DARPA Young Faculty Award (2012), and ARO Young Investigator Program (YIP) award (2012). Dr. Rondinelli has (co)-authored more than 120 peer-reviewed publications and holds 1 patent. He received a B.S. in MSE from Northwestern (2006) and a Ph.D. in Materials from the University of California, Santa Barbara (2010). From 2010-2011, he was the Joseph Katz Named Fellow in the X-Ray Science Division at Argonne National Laboratory. Prior to joining NU, he was an assistant professor at Drexel University (2011-14).