



复旦大学物理系 Colloquium

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Designing Electronic Phase Transitions with Multiple Anions

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Transition metal compounds (TMCs) offer an exciting platform for microelectronics owing to the allure of phenomena they offer. Owing to the sensitivity of their properties on (local and crystal) structure and composition, picoscale structure-property relationships are necessary to design function in TMCs. Here, I briefly overview our progress in identifying these relationships and harnessing them in heteroanionic compounds, materials comprising multiple anions of different size, electronegativity, and charge. Such heteroanionic oxynitrides, for example, may display new or enhanced responses not readily predicted from or even absent in the simpler homoanionic (oxide and nitride) compounds. Here, I show how to design rationally new heteroanionic compounds exhibiting electronic metal-insulator transitions (MITs) for highly tunable electronic materials platforms. The ability to manipulate the electronic states is key to realizing new classes of adaptive and low-power microelectronics. The strategy is to control the conducting or insulating state by structural design through inductive control over metal-metal interactions with multiple anions.



James M. Rondinelli is the Morris E. Fine Professor in Materials and Manufacturing at Northwestern University (NU) in the Materials Science and Engineering (MSE) Department and Applied Physics Program, where he leads the Materials Theory and Design Group. He serves as Co-Director of the Predictive Science and Engineering Design (PS&ED) Program and Director of Undergraduate Studies in Materials Science and Engineering. His research interests are in electronic structure theory and first-principles design of functional inorganic materials using picoscale structure-property relationships. He focuses on technical challenges and overcoming material disparities by strategically building functionality into materials through multiple tiers of materials theory, simulation, and machine-learning approaches. He has received numerous awards, including the Materials Research Society (MRS) Outstanding Young Investigator (2017), Sloan Research Fellowship in Physics (2016), and the Presidential Early Career Award for Scientists and Engineers (PECASE), among others. Rondinelli has (co)-authored more than 180 peer-reviewed publications and holds 2 patent. He is presently Member-at-Large for the American Physical Society's Division of Materials Physics. He received his Ph.D. in Materials Science 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).