

The Impact of Chemical Bonding on the Properties of ThCr₂Si₂-type Phosphides

Robert J. Cava

Department of Chemistry

Princeton University, Princeton NJ 08540 USA

Email: rcava@Princeton.EDU

Determining how crystal structure and chemical bonding influence the properties of solids is at the heart of collaborative research programs between materials physicists and solid state chemists. In some important electronic materials - the high T_c copper oxides and colossal magnetoresistance manganates for example - stoichiometry, structure, bonding, and properties are coupled to yield an almost baffling complexity of chemistry-physics relationships, while in others, such as many classical intermetallic superconductors, bonding and structure play a much less profound role. The new superconducting iron pnictides, the materials with the second highest known superconducting transition temperatures after the high T_c cuprates, appear to fall somewhere between these two limits, and thus their structure-bonding-property complexities might at first be easily overlooked. Here I will describe some of our recent work on superconductor-related cobalt-based ThCr₂Si₂-type solid solution phases as examples of the kinds of insights that structural and chemical studies can contribute to understanding the electronic properties of important electronic materials. We have found that bonding between pnictogens, which creates molecule-like dimers within what at first appear to be classical intermetallic compounds, plays a critical role in determining the observed magnetic properties.