Friday, March 3 • 2:30 PM – Biology/Physics Building, Room 130

Drawing up the Future: New Materials for Energy Application

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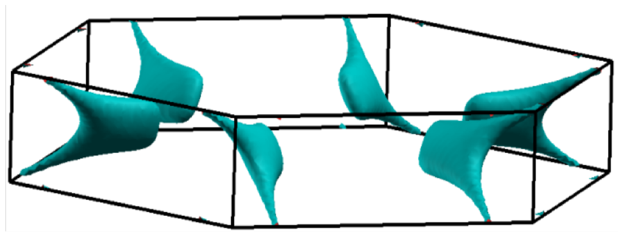
Abstract: Traditionally, the discovery of new, useful materials has proceeded by serendipity. Materials such as the $Nd_2Fe_{14}B$ permanent magnet, the piezoelectric PZT (used in diesel fuel injectors) and the Bi_2Te_3 high performance thermoelectric have been known for decades, and were discovered in the laboratory with little insight from theory. Recently, however, it has become possible to compute the relevant properties of useful materials from first principles, and thereby to design and discover new materials for energy applications. In this talk I will describe three recent findings in this field:

- The theoretical discovery [1], confirmed by pulsed magnetic field measurements at Los Alamos that the actinide ferromagnet UMn_2Ge_2 possesses an enormous magnetic anisotropy, measured at 20.7 MJ/m^3;
- The identification [2] from theory of an alloy of PZT ($PbZr_{0.5}Ti_{0.5}O_3$) with $BiZn_{0.5}Ti_{0.5}O_3$ as having some 20% higher ferroelectric polarization than PZT, and thus a potential for high piezoelectric performance; and
- The finding [3] that the silver chalcogenide semiconductor $AgBiSe_2$ may exhibit high thermoelectric performance at room temperature if properly doped *p*-type, due principally to a quasi-1D valence band feature.



A quasi-1D feature predicted to occur in the valence band of $AgBiSe_2$. Analysis indicates the feature may substantially enhance thermoelectric performance [3].

I close with an outlook for the field of "materials-by-design" and the role of theory in producing new materials.

References:

1. D.S. Parker, N. Ghimire, J. Singleton, J. D. Thompson, E. D. Bauer, R. Baumbach, D. Mandrus, L. Li, and D. J. Singh. *Phys. Rev. B* 91, 174401 (2015).

2. D.S. Parker, A. Herklotz, T. Z. Ward, M. A. McGuire, and D.J. Singh. *Phys. Rev. B* 93, 174307 (2016).

3. D.S. Parker, A. F. May, and D. J. Singh. *Phys. Rev. Appl.* 3, 064003 (2015).

Biographical Sketch: Dr. David S. Parker received his Ph.D. in Physics from the University of Southern California in 2006, studying unconventional superconductivity with Stephan Haas and the late Kazumi Maki. He then did postdoctoral work at the Max Planck Institute in Dresden, Germany from 2006 to 2008 and at the U.S. Naval Research Laboratory in Washington, D.C. from 2008 to 2010. Since 2010 he has been Staff Scientist at the Oak Ridge National Laboratory, performing theoretical work on a variety of materials for energy applications, including superconductors, thermoelectrics, magnetic materials, and ferroelectrics.ππ

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