

Time: 2:00pm, Tuesday, 2018.5.8 Location: Physics Building (Jiangwan), Room C108

## Resolving Contradictory Transport Requirements in

### **Thermoelectric Materials**

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Thermoelectric devices are used for the conversion of thermal and electrical energy. They offer a number of advantages over competing technologies including scalability to small sizes and temperature differences, simple reliable designs and often low cost. However, they have not seen wide application in energy applications due to their limited conversion efficiency. This is a consequence of the limited performance of current thermoelectric materials, which can be characterized by a dimensionless figure of merit,  $ZT=\sigma S^2T/\kappa$ . There is no known fundamental limit on ZT. However, the combination of transport parameters entering ZT is a contradictory combination that does not occur in ordinary materials. Electronic structure plays a remarkably subtle role in thermoelectric performance that can however be simply visualized in terms of iso-energy surfaces. A long sought connection is drawn between topological insulators and high ZT thermoelectrics, explaining the overlap between these two interesting materials classes. Characteristics that can be used to identify new thermoelectric compositions are discussed and an efficient computational screening method based on an electronic fitness function is presented.

#### David J. Singh:



Pushing out at the forefront of science and enabling others to do the same. Education: 1980: B.Sc (Physics), Summa cum Laude, University of Ottawa, Canada. 1985: Ph.D. (Physics), University of Ottawa, Canada. Employment: 2017-present: Curators' Professor, University of Missouri. 2015-present: Professor, Physics & Astronomy, University of Missouri. 2004-2015: Group Leader, Corporate Fellow, Oak Ridge National Laboratory. 1998-2004: Head, Theory of Functional Materials Section, Naval Res. Lab.

1990-2004: Research Physicist, Naval Research Laboratory.

1988-1990: National Research Council Associate, Naval Research Laboratory.

1985-1988: Postdoctoral Fellow of H. Krakauer, College of William & Mary.

#### Other positions:

- American Physical Society, Division of Computational Physics, Executive Committee, 2010-2013. APS Publications Oversight Committee, 2009-2012.
- Editorial Board: New Journal of Physics, Phase Transitions, Functional Materials Letters, Scientific Reports.
- Associate Editor, Materials Today Physics.

#### HIGHLIGHTS:

- Fellow of the American Physical Society.
- Fellow of the Royal Society of Chemistry.
- Conference Organization: "ESCM: Electronic Structure and Magnetism in Complex Materials" Conferences (2000 and 2002); "Quantum Complexities in Condensed Matter" (2003); "Telluride Workshop on Novel Oxides" (2005), "Novel and Complex Materials" (2005); "Fundamental Physics of Ferroelectrics" (2003, 2009, 2012); "Physics of Emergent Correlated Materials" (2013); "International Conference on Thermoelectrics" (2014).
  NBL Technology Transfer Award for Thermoelectrics" (2009)
- NRL Technology Transfer Award for Thermoelectrics Work (1998).

**Objective:** 

- 560+ Scientific Publications, 39,000+ Citations, ISI h-index of 69.
- Named Thompson Reuters "Highly Cited Researcher" (top 1% by citations).
- NRL Sigma-Xi Pure Science Award for 2000.
- E.O. Hulburt Annual Science Award, 2003 (NRL's highest scientific award).
- ORNL Directors Awards (2008 and 2009).
- Gordon Battelle Prize (2011).

