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Recent advances and challenges in thermoelectrics

Global energy issues have created a pressure to increase both the use of renewable sources of energy and the efficiency of current power generation and utilization. In the latter context thermoelectricity can play an important role in addressing the problems of energy utilization and management. The major challenge facing the thermoelectric research is to improve the efficiency which depends on dimensionless figure of merit $ZT = S^2\sigma T/\kappa$ (S is thermopower, σ is electrical conductivity, x is total thermal conductivity usually dominated by the phonons and T is the operating temperature). To achieve higher efficiency, ideas like quantum confinement, electron crystal phonon glass, nanostructuring, hierarchical structures, energy filtering, low-dimensional charge transport created by highly anisotropic electronic band structure, etc. have impacted the field of thermoelectrics during the last several decades. In this talk I will review some of the recent advances in the field and discuss how *ab initio* theoretical calculations are contributing to and clarifying these ideas. Some of the systems I will discuss are (i) thermoelectric materials with intrinsically low thermal conductivity such as layered SnSe and bulk systems with effective superlattice structure Bi(CuSe)O and Sr(AgSe)F where CuSe(AgSe) layers are sandwiched between Bi-O (Sr-F) layers; (ii) 3-dimensional systems with highly anisotropic electronic bands as in Heusler systems. I will also briefly discuss recent work on computationally guided discovery of novel thermoelelctric materials for example, n-type Zintl compounds.

Recent Publications

1. D Bilc et al. (2004) Resonant States in the Electronic Structure of High Performance Thermoelectrics $AgPb_mSbTe_{2+m}$; the role of Ag-Sb microstructures. Phys. Rev. Letters. 93(14):146403.
2. S Ahmad et al. (2006) *Ab initio* study of deep defect states in narrow band-gap semiconductors: group iii impurities in PbTe. Phys. Rev. Letters: 96(5):056403.
3. K Hoang et al. (2007) Atomic ordering and gap formation in Ag-Sb based ternary chalcogenides. Phys. Rev. Letters. 99(15):156402.
4. Dat T Do and S D Mahanti (2014) Bonds, bands, and bandgaps in tetrahedrally bonded ternary compounds: the role of group V lone pairs. Journal of Physics and Chemistry of Solids. 75(4):477-485.
5. Y O Ciftci and S D Mahanti (2016) Electronic structure and thermoelelctric properties of half-Heusler compounds with eight valence electron count – KScX (X=C and Ge). Journal of Applied Physics. 119(14):145703.

Biography

Subhendra Dev Mahanti obtained his BSc from Utkal University in 1961; MSc from Allahabad University in 1963; PhD in Theoretical Condensed Matter Physics from the University of California, Riverside (USA) in 1968. After two years at Bell Telephone Laboratories, he joined Michigan State University in 1970, where he has been a Full Professor since 1982 and is currently an Emeritus Professor. His research is in the area of magnetism, high T_c superconductors, multi-ferroics, physical systems showing colossal magnetic resistance, thermoelectrics, and topological insulators. He has published nearly 300 papers in reputed journals.

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