

EFRC: SOLID-STATE SOLAR THERMAL ENERGY CONVERSION CENTER (S³TEC) UPDATED: AUGUST 2016

AWARDS: \$17.7M (August 2009 – July 2014); \$12.8M (August 2014 – July 2018) WEBSITES: http://science.energy.gov/bes/efrc/centers/s3tec/; https://s3tec.mit.edu/ TEAM: MIT (Lead): Gang Chen (Director), Evelyn N. Wang (Associate Director), Mildred Dresselhaus, Marin Soljacic, Keith Nelson, Yang Shao-Horn, Caroline Ross, Nicolas Hadjiconstantinou, Alexie Kolpak, Liang Fu (Seed Fund); Boston College: David Broido; University of Houston: Zhifeng Ren; Northwestern University: Jeffrey Snyder; Duke University: Olivier Delaire; University of Missouri: David Singh; Brookhaven National Laboratory: Yimei Zhu

SCIENTIFIC MISSION AND APPROACH

The goals of S³TEC are to advance fundamental science and to develop materials for harnessing heat from the Sun and terrestrial sources and converting this heat into electricity via solid-state thermoelectric, thermogalvanic and thermophotovoltaic technologies. The S³TEC research forms the foundation for understanding thermodynamic and transport processes of photons, phonons, electrons, ions and spins as well as their interactions that increase efficiency of the energy conversion processes. S³TEC advances new materials for the solid-state energy conversion schemes and demonstrates new concepts via experiments. The research is organized around three major thrusts:

- 1) <u>Electron, phonon, and ion transport</u>: Develop tools to predict and probe electron, phonon, and ion transport properties that are of vital importance to thermoelectric and thermogalvanic energy conversion.
- 2) <u>Thermoelectric and thermogalvanic materials</u>: Design, synthesize, and characterize materials to improve the efficiency of thermoelectric and thermogalvanic energy conversion.
- 3) <u>High temperature photonics and thermophotovoltaics</u>: Discover new ways to manipulate photon absorption, emission and reflection to develop high-performance selective absorbers and emitters that are stable at high temperatures for thermophotovoltaic and thermoelectric energy conversion.

SELECTED SCIENTIFIC ACCOMPLISHMENTS

- Invented spectroscopy techniques to measure phonon mean free path distributions in thermoelectric materials on an optical table.
- Advanced first-principle simulation techniques to enable *ab initio* accurate predictions of all thermoelectric transport properties.
- Observed phonon localization in heat conduction and predicted phonon hydrodynamic modes in 2D materials.
- Discovered semiconducting half-heuslers with highest power factor, achieved high thermoelectric figure of merit in SnSe-based single crystals (peak ZT ~ 2).
- Made first experimental observation of Weyl points in photonics crystals and of a ring of exceptional points spawned from a single Dirac cone, connecting Dirac physics and non-Hermitian physics.
- Proof-of-principle experiments demonstrated solar thermoelectric generators with efficiencies at 4.6% without optical concentration and 7.4% with optical concentration.
- Proof-of-principle experiments demonstrated solar thermophotovoltaic efficiency at 6.8%.
- Based on fundamental insights into tailoring high-temperature thermal radiation, invented a new type of incandescent light bulb with efficiency that can surpass that of a light emitting diode.





S³TEC research, from left: Weyl points demonstration in photonic crystals; Thermoelectric (TE) generator prototype; novel highefficiency incandescent light bulb; phonon mean free path measurements (MFP) results for various TE materials; first-principles calculations and neutron and electron beam probing of phonon transport; SEM image of a nanodot structure used in phonon MFP spectroscopy.

IMPACT

- S³TEC students and post-docs are sought-after: 15 of 39 alumni have accepted faculty positions.
- Weyl point in photonic crystals was one of the 2015 Physics World's top ten breakthrough and one of the 2015 American Physical Society's Highlights of the Year; thermally regenerative electrochemical cycles was one of top 10 World Changing Ideas by the Scientific American Magazine in 2014; angular selectivity was one of top 100 science stories of 2014 by Discover Magazine.
- S³TEC organized <u>OSA Incubator on Fundamental Limits of Optical Energy Conversion</u>, featuring speakers from S³TEC and other EFRCs including LMI, CASP and CNGMD. As a result of the event discussions, S³TEC published a <u>Roadmap on Optical Energy Conversion</u> in the IOP Journal of Optics.
- S³TEC obtained follow-up funding from DOE for the development of high-efficiency solar TE generators (award DE-EE0005806, 2012-2015).
- S³TEC basic research has led to practical applications, as indicated by multiple patent applications and one spin-off company, **Thermoaura Inc.**, which was founded in 2011 and markets high-performance thermoelectric nanomaterials pioneered by the S³TEC researchers: <u>http://thermoaura.com/</u>.

PUBLICATIONS AND INTELLECTUAL PROPERTY

As of May 2016, S³TEC had published 313 peer-reviewed publications cited over 11,600 times and filed 46 disclosures, 40 US patent applications, and 27 foreign patent applications. 10 patents have been issued. A selection of highly cited papers are:

- Zebarjadi, M. *et al.* Perspectives on thermoelectrics: from fundamentals to device applications. *Energy & Environmental Science* **5**, 5147, doi: <u>10.1039/c1ee02497c</u> (2012). [**353 citations**]
- Kraemer, D. *et al.* High-performance flat-panel solar thermoelectric generators with high thermal concentration. *Nature Mater*ials **10**, 532–538, doi:<u>10.1038/nmat3013</u> (2011). [**334 citations**]
- Lan, Y. *et al.* Enhancement of thermoelectric figure-of-merit by a bulk nanostructuring approach. *Advanced Functional Materials* **20**, 357–376, doi: <u>10.1002/adfm.200901512</u> (2010). [**330 citations**]
- Esfarjani, K., Chen, G. & Stokes, H. Heat transport in silicon from first-principles calculations. *Physical Review B* **84**, doi: <u>10.1103/PhysRevB.84.085204</u> (2011). [**234 citations**]
- Liu, W. *et al.* Recent advances in thermoelectric nanocomposites. *Nano Energy* **1**, 42–56, doi:<u>10.1016/j.nanoen.2011.10.001</u> (2012). [**206 citations**]
- Yan, X. *et al*. Experimental studies on anisotropic thermoelectric properties and structures of n-type Bi₂Te_{2.7}Se_{0.3}. *Nano Letters* **10**, 3373–3378, doi: <u>10.1021/nl101156v</u> (2010). [**201 citations**]
- Mehta, R. J. *et al*. A new class of doped nanobulk high-figure-of-merit thermoelectrics by scalable bottom-up assembly. *Nature Materials* **11**, 233–240, doi:<u>10.1038/nmat3213</u> (2012). [**198 citations**]
- Wei, Y. *et al*. The nature of strength enhancement and weakening by pentagon–heptagon defects in graphene. Nature Materials **11**, 759–763, doi: <u>10.1038/nmat3370</u> (2012). [**184 citations**]
- Minnich, A. *et al.* Thermal conductivity spectroscopy technique to measure phonon mean free paths. *Physical Review Letters* **107**, 095901, doi: <u>10.1103/PhysRevLett.107.095901</u> (2011). [**177 citations**]
- Delaire, O. *et al*. Giant anharmonic phonon scattering in PbTe. *Nature Materials* 10, 614–619, doi: <u>10.1038/NMAT3035</u> (2011). [171 citations]