School of Natural Sciences
Physics Colloquium Series

UCMERCED

Solid-State Chemistry in Energy Efficiency: Lighting Phosphors and Thermoelectric Materials

By Ram Seshadri

Materials Department and Department of Chemistry and Biochemistry
Materials Research Laboratory
University of California, Santa Barbara

Date: 09/30/16 **Time: 10:30 AM** **Location: COB 267**

For More Information Contact: Linda Hirst, lhirst@ucmerced.edu

Abstract:

In the first part, I will address phosphors that play a key role in the now almost-mature solid-state white-lighting technologies based on combining a III-nitride-based near-UV or blue solid-state light source with down-conversion to longer wavelengths.[1] Almost all widely used phosphors comprise a crystalline oxide, nitride, or oxynitride host that is appropriately doped with either Ce3+ or Eu2+. Optical excitation into these states and concomitant reemission can be tuned into the appropriate regions of the visible spectrum by the crystal these ions are hosted in. Experimental studies of some of the best phosphor materials, employing state-of-the-art structural tools, have yielded guidelines for what are desirable structural features. We find that a useful sorting diagram for efficient hosts with high quantum yield has the band gap of the host – readily calculated with high reliability using hybrid functionals in DFT – as one of the axes, and the calculated Debye temperature as the other axis.[2]

In the second part, I will describe the creation of a large database of thermoelectric materials prepared by abstracting information from over 100 publications. Appropriate visualization of the data immediately allows certain insights to be gained with regard to the property space of plausible thermoelectric materials. The Herfindahl–Hirschman index – a commonly accepted measure of market concentration and monopoly – has been calculated from geological data (known elemental reserves) and geopolitical data (elemental production) for much of the periodic table. The visualization strategy employed allows rapid sorting of thermoelectric compositions with respect to important issues of elemental scarcity and supply risk.[3]

[1] N. C. George, K. A. Denault, and R. Seshadri, Phosphors for solid-state white lighting, Annu. Rev. Mater. Res. 43 (2013) 481–501.

[2] J. Brgoch, S. P. DenBaars, and R. Seshadri, Proxies from ab-initio calculations for screening efficient Ce3+ phosphor hosts, J. Phys. Chem. C 117 (2013) 17955–17959.

[3] M. W. Gaultois, T. D. Sparks, C. K. H. Borg, R. Seshadri, W. D. Bonificio, and D. R. Clarke, A data-driven review of thermoelectric materials: Performance and resource considerations, Chem. Mater. 25 (2013) 2911–2920.

Bio:

Ram Seshadri received his Ph.D. in 1995 from the Indian Institute of Science in Bangalore. After some years as a post-doctoral fellow in the CNRS in Caen, France, and in the University of Mainz, Germany, he joined the faculty of the Indian Institute of Science in 1999. He moved to the Materials Department, UCSB in 2002 as an Assistant Professor, and was promoted to Associate Professor in 2006 and Professor in 2008. In Fall 2007, he also joined the faculty in the Department of Chemistry and Biochemistry. The research currently being pursued addresses magnetic phenomena in insulating oxides, half-metallic ferromagnetism, magnetic nanocomposites, catalytic oxides and carbides, the structure and electronic structure of polar and semiconducting materials (bulk as well as nano), luminescent materials for solid state lighting, high refractive index materials, and conducting nanowires.