UC San Diego
JACOBS SCHOOL OF ENGINEERING
NanoEngineering

Zhenbin Wang Dissertation Defense
NanoEngineering Ph.D. Candidate
Materials Virtual Lab
Tuesday, March 6, 2018
1:00p.m.
Jack Keil Wolf Auditorium (CMRR)

"Design and Optimization of Phosphors for Solid-State Lighting using First-Principles Calculations"

PI: Dr. Shyue Ping Ong

Abstract: The discovery of novel phosphors is key to the development of highly efficient and environmental friendly light-emitting diodes (LED) for solid-state lighting. The aim of this thesis is to use high-throughput first principles calculations to gain fundamental insights into structure-property relationships in phosphor materials and apply these insights to accelerate the discovery and optimization of novel phosphors. In the first project, we developed a quantitative descriptor for narrow-band Eu^{2+}-activated emission. Phosphors with narrow-band emission are a critical component for high brightness LEDs and liquid crystal display backlighting with wide color gamut. Incorporating this descriptor into a high-throughput screening, we identified five promising new Eu^{2+}-activated red-emitting nitride phosphors. In the second project, we performed a systematic investigation of structure-composition-property relationships in Eu^{2+}-activated β-SiAlON, one of the most promising narrow-band green phosphors. We first identified the most energetically favorable structure for β-SiAlON:Eu^{2+} and then studied the effect of oxygen content and Eu^{2+} activator concentrations on important photoluminescence (PL) properties. The insights obtained provide useful guidelines to optimize the PL performance of β-SiAlON, which have been independently verified by other researchers. In the final project, we developed an approach to discover new oxide phosphors by mining unexplored chemistries with data-driven structure prediction and high-throughput screening. We discovered a novel, earth-abundant phosphor host, Sr_2LiAlO_4, which was successfully synthesized and integrated into prototype LEDs with high color quality.

Biosketch: Zhenbin Wang was born in Anyang, China. He received his B.E. from Harbin Institute of Technology in 2011 and M.E. from University of Science and Technology of China in 2014.