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

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**Abstract:** The discovery of novel phosphors is key to the development of highly efficient and environmentally 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$_2$LiAlO$_4$, 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.