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## Unraveling luminescence behavior of 3d<sup>3</sup> ions in solids: Navigating from crystal-field theory to first-principles analysis

*School of Optoelectronic Engineering, Chongqing University of Posts and  
Telecommunications, Chongqing 400065, China*

**Chong-Geng Ma**

**E-mail: cgma.ustc@gmail.com**

Phosphors activated by 3d<sup>3</sup> ions are increasingly gaining prominence in the field of solid-state lighting due to their efficacy as red photon emitters. This presentation aims to underscore pivotal factors crucial for designing commercially viable red-emitting phosphors. Our focus lies in comprehending the electronic energy levels of 3d<sup>3</sup> ions in both free-state and crystal-field environments, utilizing a semi-empirical data mining technique. Moreover, we propose a robust first-principles approach to enhance the description of excited <sup>2</sup>E and <sup>4</sup>T<sub>2</sub> states in 3d<sup>3</sup> ions, enabling accurate predictions of the structural, electronic, and optical properties of red-emitting phosphors doped with these ions. This proposed calculation scheme has demonstrated success in Mn<sup>4+</sup>-doped K<sub>2</sub>SiF<sub>6</sub> and Cr<sup>3+</sup>-doped Ca<sub>3</sub>Y<sub>2</sub>Ge<sub>3</sub>O<sub>12</sub> phosphors. Additionally, it distinctly unveils the physical-pressure/chemical-stress induced excited-state crossover in K<sub>3</sub>MF<sub>6</sub>:Cr<sup>3+</sup> (M=Al, Ga) from a first-principles perspective. Furthermore, we delve into the thermal stabilities of the Mn<sup>4+</sup>/Cr<sup>3+</sup> emissions within the studied hosts, analyzing their thermal activation energies for the first time via the calculated configuration coordinate diagrams. Ultimately, based on these findings, we offer practical recommendations for fine-tuning the emission wavelengths and intensities of Mn<sup>4+</sup>/Cr<sup>3+</sup>-doped red-emitting phosphors.



### **Short Bio:**

**Chong-Geng Ma** earned his PhD from University of Science and Technology of China in 2008. Currently, he is a foreign member of the National Academy of Sciences of Tajikistan, the vice chairman of the LDM division in ECS, an associate editor of Optical Materials (Elsevier), and a full professor and director at CQUPT-BUL Innovation Institute, Chongqing University of Posts and

Telecommunications, China.