

Probing the Electronic Structure and Luminescence Mechanisms of BaSiP₃N₇:Eu²⁺ Using DFT and Synchrotron-Based Spectroscopy.
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The development of high-efficiency light-emitting diodes (LEDs) relies on advanced luminescent materials that enhance their performance. BaSiP₃N₇:Eu²⁺ has emerged as a promising phosphor due to its strong luminescence properties. To gain deeper insight into its electronic and optical behavior, we employed a combination of experimental techniques, including X-ray absorption spectroscopy (**XAS**), X-ray emission spectroscopy (**XES**), resonant inelastic X-ray scattering (**RIXS**), and X-ray excited optical luminescence (**XEOL**), complemented by density functional theory (**DFT**) calculations.

Our study reveals key electron transition mechanisms, notably the **5d → 4f** transition of Eu²⁺, which serves as the primary indicator of luminescence efficiency. Additionally, we examine charge transfer effects, thermal quenching mechanisms, energy transfer pathways, and defect impurities arising from material synthesis in BaSiPN:Eu²⁺, providing deeper insight into the factors that govern its luminescence performance. These findings deepen our understanding of the electronic and optical properties of BaSiP₃N₇:Eu²⁺, guiding its optimization as a high-performance phosphor for LED applications.