

## Accepted Manuscript

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PII: S1385-8947(18)31754-6  
DOI: <https://doi.org/10.1016/j.cej.2018.09.036>  
Reference: CEJ 19875

To appear in: *Chemical Engineering Journal*

Received Date: 12 June 2018  
Revised Date: 4 September 2018  
Accepted Date: 6 September 2018

Please cite this article as: J. Xiang, J. Zheng, Z. Zhou, H. Suo, X. Zhao, X. Zhou, N. Zhang, M.S. Molochev, C. Guo, Enhancement of red emission and site analysis in  $\text{Eu}^{2+}$  doped new-type structure  $\text{Ba}_3\text{CaK}(\text{PO}_4)_3$  for plant growth white LEDs, *Chemical Engineering Journal* (2018), doi: <https://doi.org/10.1016/j.cej.2018.09.036>



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# Enhancement of Red Emission and Site Analysis in $\text{Eu}^{2+}$ Doped New-Type Structure $\text{Ba}_3\text{CaK}(\text{PO}_4)_3$ for Plant Growth White LEDs

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## Abstract

A novel compound  $\text{Ba}_3\text{CaK}(\text{PO}_4)_3$  (BCKP) with new-type structure was synthesized and its structure was determined by X-ray diffraction Rietveld refinement, in which crystal structure consists of  $\text{Ba}_1\text{O}_9$ ,  $\text{Ba}_2\text{O}_{12}$ ,  $\text{Ba}_3\text{O}_9$ ,  $\text{CaO}_8$  and  $\text{KO}_{10}$  polyhedra, that's five cationic sites. As a phosphor host,  $\text{Eu}^{2+}$  doped BCKP emits cold white light with about 90% quantum efficiency (QE) through entering different cationic sites. Based on the results of refinement, three  $\text{Eu}^{2+}$  luminescence centers in sites Ca, Ba2 and K were clearly assigned in  $\text{Eu}^{2+}$  solely doped BCKP by the time-resolved emission spectra (TRES), Van Uitert equation, but the emissions of  $\text{Eu}^{2+}$  at Ba1 and Ba3 sites are not easy to be determined for the same coordination number (CN). According to their different spatial distribution of the coordinated atoms, the *first-principles calculation* was used to compute the *d* orbital splitting energy of  $\text{Eu}^{2+}$  ions in Ba1 and Ba3 sites to accurately distinguish the ambiguous luminescence centers. In order to meet the requirement of plant growth

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