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New green phosphor $Ba_3Si_6O_{12}N_2$:Eu for white LED: crystal structure and optical properties MASAYOSHI MIKAMI, KYOTA UHEDA, SATOSHI SHIMOOKA, HIROYUKI IMURA, NAOTO KIJIMA, Mitsubishi Chemical Group Science and Technology Research Center, Inc. — A new oxynitride, $Ba_3Si_6O_{12}N_2$, has been synthesized. The crystal structure has been successfully determined by close collaboration between experiment and first-principles band calculation based on density functional theory. This compound doped with Eu exhibits intense green photoluminescence with high color purity under near-ultraviolet to blue light excitation. It has much less thermal quenching than other green phosphor $(Ba,Sr,Eu)_2SiO_4$. Hence $(Ba,Eu)_3Si_6O_{12}N_2$ appears promising green phosphor for white LED backlight for display. The atomic/electronic structure is discussed in comparison with a similar oxynitride $Ba_3Si_6O_9N_4$, which could not become efficient phosphor by doping Eu due to strong thermal quenching at room temperature. The optical properties of these compounds have been interpreted from theoretical and crystallographic viewpoint.

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