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Computational nano-material design of exotic luminescent materials based upon europium doped gallium nitrides AKIRA MASAGO, TETSUYA FUKUSHIMA, Graduate School of Engineering Science, Osaka University, KAZUNORI SATO, Graduate School of Engineering, Osaka University, HIROSHI KATAYAMA-YOSHIDA, Graduate School of Engineering Science, Osaka University — Eu-doped GaN has attracted much attention, because the red light luminescence ability provides us with expectations to realize monolithic full-color LEDs, which work on seamless conditions such as substrates, electrodes, and operating bias voltages. Toward implementation of multifunctional activity into the luminescent materials using the spinodal nano-structures, we investigate atomic configurations and magnetic structures of the GaN crystal codoped with Eu, Mg, Si, O, and/or the vacancies using the density functional method (DFT) calculations. Our calculations show that the impurity clusterized distributions are energetically favorable more than the homogeneous distribution. Moreover, analyses of the formation energy and binding energy suggest that the clusterized distributions are spontaneously formed by the nano-spinodal decomposition. Though the host matrix has no magnetic moments, the cluster has finite magnetic moments, where Zener's p-f exchange interaction works between the Eu f-state and the nearby N p-states.

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