AB INITIO CALCULATION OF THE ELECTRONIC TRANSITIONS OF Er\(^{3+}\) DOPED INTO GaN

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As a potential application in optical communications, the 1.54 \(\mu\)m photoluminescence (\(^4I_{13/2} \rightarrow ^4I_{15/2}\) intra-4f shell emissions) of Er\(^{3+}\) doped in the semiconductor GaN has been studied extensively since 1983. Few \textit{ab initio} calculations touched this system before because of the difficulties dealing with the large number of electrons and the significant relativistic effects related to Er\(^{3+}\). Based on relativistic effective core potentials, spin-orbit configuration interaction calculations have been performed on this system. The study of the wave function character and energy of both the ground and excited states of ErN\(_4^{0-}\) plus the computation of the transition moments between the states gives a better understanding of the experimental results.