THEORETICAL STUDY OF 1.54 µm ELECTRONIC TRANSITIONS OF Er³⁺ DOPED INTO GaN

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A strong interest in 1.54 μ m photoluminescence (${}^{4}I_{13/2} \rightarrow {}^{4}I_{15/2}$ intra-4f shell emissions) of Er^{3+} doped into the semiconductor GaN can be traced back to the early 1980s because of its efficient transmission and temperature stability in semiconductor-based fibers, which make its application in optical communications promising. *Ab initio* spin-orbit configuration interaction calculations based on relativistic effective core potentials were carried out in our current work to effectively treat the large number of electrons and significant relativistic effects related to Er^{3+} . The study of the wave function character and energy of both the ground and excited states of a series of Er^{3+} -centered clusters and the calculations of the transition moments between the states help us explain the experimental results.