THEORETICAL STUDY OF Er^{3+} DOPED IN SEMICONDUCTOR GaN BASED ON RELATIVISTIC QUANTUM CHEMICAL METHOD

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The 1.54 μm photoluminescence ($^4I_{13/2} \rightarrow {}^4I_{15/2}$ intra-4f shell emissions) of Er^{3+} doped in the semiconductor GaN has attracted interest for a long time, because of the potential application in optical communications due to its efficient transmission and temperature stability in semiconductor-based fibers. In our current research, we use *ab initio* spin-orbit configuration interaction calculations with relativistic effective core potentials to study the wave function character and energy of both the ground and excited states of ErN_4^{9-} aiming to compare the calculated transition frequency between those states with the available experimental data. In this calculation, ErN_4^{9-} has a local tetrahedral symmetry in the GaN crystal. The transition moments will be computed as well to understand the interactions giving a non-zero value.