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

YANG YANG and RUSSELL M. PITZER, *Department of Chemistry, The Ohio State University, Columbus, OH 43210*.

As a potential application in optical communications, 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 been studied extensively since 1983. Few *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^{9-} plus the computation of the transition moments between the states gives a better understanding of the experimental results.