

## AB INITIO CALCULATION OF THE ELECTRONIC TRANSITIONS OF $\text{Er}^{3+}$ 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  $\mu\text{m}$  photoluminescence ( $^4I_{13/2} \rightarrow ^4I_{15/2}$  intra-4f shell emissions) of  $\text{Er}^{3+}$  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  $\text{Er}^{3+}$ . 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  $\text{ErN}_4^{9-}$  plus the computation of the transition moments between the states gives a better understanding of the experimental results.