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First-principles Study of Hydrogen depassivation of Mg acceptor by Be in GaN QIMING ZHANG, XIAO WANG, University of Texas at Arlington, CHIHSIANG WANG, National Taitung University, Taiwan — The process of hydrogen depassivation of the acceptor by can convert the as-grown high-resistivity -doped into a - conducting material. A first-principles study on the process will be presented. The formation energies of various complex of impurities and point defects have been calculated and compared. The diffusion barriers of the hydrogen atom in the doped GaN have been obtained by the Nudge-Elastic-Band method. The results explain successfully the experimental observation that the hole concentration has been significantly enhanced in a Be-implanted Mg-doped GaN.

Qiming Zhang
University of Texas at Arlington

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