

Abstract Submitted
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The delocalized nature of holes in (Ga, N) cluster doped ZnO¹

MUHAMMAD N. HUDA, University of Texas at Arlington, YANFA YAN, National Renewable Energy Laboratory, MOWAFAK M. AL-JASSIM, National Renewable Energy Laboratory — (Ga, N) cluster-doping in ZnO has been considered as a valid approach to enhance the p-type doping of ZnO. So far, the argument on the enhancement is based on the reduction of dopant formation energy and ionization energy. Here we present spin-polarized density functional theory calculation to reveal that in (Ga, N) cluster doping of ZnO, a hole state created by a (Ga, N) cluster contains the contribution from all N atoms in the cluster, meaning a more delocalized nature of the hole as compared to the case of mono N doping of ZnO. Our results explain from the electronic point of view why (Ga, N) cluster doping enhances the p-type doping of ZnO. We will compare both LDA+U and hybrid density functional calculations.

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