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The Electronic Properties of Native Point Defects at ZnO Surfaces and Interfaces[1]

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Despite nearly sixty years of research, several fundamental issues surrounding ZnO remain unresolved. Among the key roadblocks to ZnO optoelectronics have been the difficulty of p-type doping and the role of compensating native defects. Oxygen vacancies (V_O), Zn interstitials (Zn_I), and residual impurities such as H, Al, Ga, and In are reported to be donors in ZnO, while Zn vacancies (V_{Zn}) are considered to be acceptors. Electrically active complexes of V_O, Zn_I, and V_{Zn} can also exist. Although their impact on free carrier compensation and recombination is recognized, the physical nature of the donors and acceptors dominating carrier densities in ZnO and their effects on carrier injection at contacts is unresolved. The impact of these electronic states on ZnO carriers at the nanoscale is only now being explored. We can now address these issues using a combination of depth-resolved and scanned probe techniques. Taken together, we clearly identify the optical transitions and energies of V_{Zn} and V_{Zn} clusters, effects of annealing on their spatial distributions in ion-implanted ZnO, and how V_{Zn} and V_{Zn} clusters modify the near- and sub-surface carrier densities. Indeed, these native point defects can directly impact the activation of extrinsic dopants. We have now discovered that nanostructures form spontaneously on ZnO polar surfaces and create sub-surface V_{Zn} locally because of Zn diffusion that feeds the nanostructure growth. Overall, this work reveals the interplay between ZnO electronic defects, polarity, and surface nanostructure.

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[2] D. Doutt, H. L. Mosbacker, G. Cantwell,J. Zhang, J. J. Song, and L. J. Brillson, "Impact of near-surface defects and morphology on ZnO luminescence," Appl. Phys. Lett. **94**, 042111 (2009).

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