Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Vacancy-assisted migration of group-III impurities in ZnO[1]
DANIEL STEIAUF, JOHN L. LYONS, ANDERSON JANOTTI, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara, CA 93106 — Zinc oxide is a wide-band-gap material used as transparent conductor. As grown it often shows n-type conductivity, probably due to impurity contamination. High electron concentrations can be achieved by intentional doping with group-III elements, a process that usually involves annealing. It is thus important to understand the diffusion properties of the dopants. We perform first-principles calculations for the vacancy-assisted migration process of Al, Ga and In in ZnO, using both standard density functionals and hybrid functionals to correct the underestimated band gap. Indium induces the largest distortions in the lattice and has the highest formation energy. Its migration barrier to a neighboring Zn vacancy is the lowest. Al shows the highest barrier and thus has the best thermal stability. From the calculated migration barriers and formation energies, we determine diffusion activation energies and estimate annealing temperatures. The results are compared with recent experiments.

[1]This work was supported by Saint Gobain Research and by the NSF MRSEC Program.

Daniel Steiauf
Materials Department, University of California, Santa Barbara, CA 93106

Date submitted: 18 Nov 2010 Electronic form version 1.4