Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

A pathway to p-type wide-band-gap semiconductors[1] ANDERSON JANOTTI, CHRIS G. VAN DE WALLE, Materials Department, University of California Santa Barbara — The development of solid-state ultraviolet-light sources in the form of light-emitting diodes and laser diodes to replace mercury lamps and bulky gas lasers is currently hindered by doping issues in wide-band-gap semiconductors such as AlN, ZnO, and ZnMgO alloys. While n-type AlN, ZnO, and ZnMgO can be achieved by using traditional doping concepts, i.e. swapping host atoms for impurities with an extra valence electron, p-type is still a major challenge. Based on first-principles calculations we devise an alternative approach to p-type doping in AlN, ZnO, and ZnMgO. Instead of searching for acceptors on the left of the host atoms in the periodic table, we propose to search on the far right. We find that F placed at interstitial sites in AlN, ZnO, and ZnMgO acts as a shallow acceptor, leaving a hole in an effective-mass state near the valence-band maximum. We discuss the stability of F impurities, and propose a procedure to selectively introduce F in the interstitial lattice sites of the above wide-band-gap semiconductors.

[1]Work supported by the NSF MRSEC Program under Grant No. DMR05-20415 and by the UCSB Solid State Lighting and Energy Center.

Anderson Janotti
Materials Department, University of California Santa Barbara

Date submitted: 23 Nov 2009 Electronic form version 1.4