Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Role of self-trapping in luminescence and p-type conductivity of wide-band-gap oxides[1] JOEL VARLEY, Stanford University, ANDERSON JANOTTI, University of California, Santa Barbara, CESARE FRANCHINI, University of Vienna and Center for Computational Materials Science, CHRIS VAN DE WALLE, University of California, Santa Barbara — Using hybrid functional calculations, we investigate the behavior of holes in the valence band of a range of wide-band-gap oxides including ZnO, MgO, In_2O_3, Ga_2O_3, Al_2O_3, SnO_2, SiO_2, and TiO_2. We find that, due to the orbital composition of the valence band, holes tend to form localized small polarons with characteristic lattice distortions, even in the absence of defects or impurities. These self-trapped holes (STHs) are energetically more favorable than delocalized, free holes in the valence band in all materials but ZnO and SiO_2. Based on calculated optical absorption and emission energies we show that STHs provide an explanation for the luminescence peaks that have been observed in many of these oxides. Additionally, we demonstrate that polaron formation prohibits p-type conductivity in this class of materials.

[1]This work was supported by the NSF MRSEC Program (DMR05-20415).

Joel Varley
Stanford University

Date submitted: 29 Nov 2012 Electronic form version 1.4