Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Free-carrier effects on electronic and optical properties of binary oxide semiconductors[1] ANDRE SCHLEIFE, Lawrence Livermore Natl. Lab. and Univ. of Illinois, CLAUDIA ROEDL, LSI, Ecole Polytechnique, CNRS, CEA, Palaiseau, France — While there is persistent interest in oxides, e.g., for semiconductor technology or optoelectronics, it remains difficult to achieve n-type and p-type doping of one and the same material. At the same time, higher and higher conductivities are reported for both types of doping individually. Hence, it is important to understand the corresponding influence of free carriers on electronic structure and optical properties. Modern electronic-structure calculations, based on hybrid exchange-correlation functionals and the GW approximation, were performed for n-type (ZnO, CdO, SnO_2) and p-type (MnO, NiO) binary oxides. We use these results to analyze the influence of free carriers by computing contributions that increase (Burstein-Moss shift) or reduce (electron-electron interaction and ionized-impurity scattering) the band gaps as a function of free-carrier concentration. We also compute the carrier-concentration dependence of effective electron and hole masses and compare to experimental data. For n-type ZnO we compute optical absorption spectra by means of a recent extension of the Bethe-Salpeter framework. This allows us to take excitonic effects as well as the influence of free carriers on the electron-hole interaction into account.

[1]Prepared by LLNL under Contract DE-AC52-07NA27344

Andre Schleife
Dept. of Mat. Sci. and Eng., Univ. of Illinois Urbana-Champaign

Date submitted: 15 Nov 2013 Electronic form version 1.4