Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Optical properties of group-II oxides – excitons and absorption in MgO, ZnO and CdO ANDRÉ SCHLEIFE, CLAUDIA RÖDL, FRANK FUCHS, FRIEDHELM BECHSTEDT, Institut fuer Festkoerpertheorie und -optik, Friedrich-Schiller-Universitaet and European Theoretical Spectroscopy Facility (ETSF) — ZnO is a material that has been very attractive for researchers for many decades by now. However, recently also alloys and heterostructures with other group-II oxides are becoming more and more interesting. Together with MgO or CdO the tuning of electronic and optical properties becomes possible with potential applications for optoelectronic devices in the blue or UV spectral region. For the three materials we study the influence of excitonic effects on the dielectric function in the region of interband transitions and on the electron-hole binding near the absorption edge by solving the Bethe-Salpeter equation. As starting point we compute the electronic structure using a GGA+U approach. The U is chosen to widely reproduce more sophisticated HSE03+GW calculations. We combine two efficient approaches to calculate the spectrum and bound excitonic states, using a large number of **k**-points in combination with hybrid **k**-point meshes to ensure convergence. We find good agreement of our challenging *ab initio* calculations with experimental absorption spectra as well as values for the binding energies.

Andre Schleife
Institut fuer Festkoerpertheorie und -optik, Friedrich-Schiller-Universitaet
and European Theoretical Spectroscopy Facility (ETSF)

Date submitted: 30 Nov 2007 Electronic form version 1.4