Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Optical absorption in degenerately doped semiconductors: Mott transition or Mahan excitons? ANDRÉ SCHLEIFE, Lawrence Livermore National Laboratory, CLAUDIA RÖDL, KARSTEN HANNEWALD, FRIEDHELM BECHSTEDT, Institut fuer Festkoerpertheorie und -optik, Friedrich-Schiller-Universitaet Jena — In the exploration of material properties, parameter-free calculations are a modern, sophisticated complement to cutting-edge experimental techniques. *Ab-initio* calculations are now capable of providing a deep understanding of the interesting physics underlying the electronic structure and optical absorption, e.g., of the transparent conductive oxides. Due to electron doping, these materials are conductive even though they have wide fundamental band gaps. The degenerate electron gas in the lowest conduction-band states drastically modifies the Coulomb interaction between the electrons and, hence, the optical properties close to the absorption edge. We describe these effects by developing an *ab-initio* technique which captures also the Pauli blocking and the Fermi-edge singularity at the optical absorption onset, that occur in addition to quasiparticle and excitonic effects. We answer the question whether free carriers induce an excitonic Mott transition or trigger the evolution of Wannier-Mott excitons into Mahan excitons. The prototypical n-type zinc oxide is studied as an example.

Friedhelm Bechstedt
Institut fuer Festkoerpertheorie und -optik,
Friedrich-Schiller-Universitaet Jena

Date submitted: 29 Nov 2011 Electronic form version 1.4