Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Nickel and Chromium doped ZnO: electronic, magnetic, and optical properties studied via first-principles calculations. LUISA SCOLFARO, Texas State University, NAIARA CASTRO, Universidade Federal de Uberlandia, PABLO BORGES, Universidade de Vicosa, RENATA LIMA, Universidade Federal de Uberlandia — As one of the most important transition metal oxide semiconductors, ZnO has not only been widely used, in As one of the most important transition metal oxide semiconductors, ZnO has not only been widely used, in optoelectronics, gas sensors and solar cells, but it has shown potential application for next-generation resistive nonvolatile memories. In this work, we study the electronic and magnetic properties of Nickel and Chromium doped ZnO, as well as Ni and Cr codoped ZnO using first-principles band structure calculations, performed within Density Functional Theory. We use the mBJ+U_{Zn} approach which allowed to better describe the electronic structure of pure zinc oxide, providing a gap value in excellent agreement with experiment. The 3d related levels arising from the Ni and Cr impurities are found to lie close to the top of the valence band and in the gap region, respectively, being responsible for a reduction in the ZnO bandgap. From the band structure calculations, we obtained the real and imaginary parts of the frequency-dependent complex dielectric function for pure and doped systems. Our findings for the dielectric function, electrical conductivity and loss function are discussed in regard to device applications. Comparisons with results on doped samples grown using hydrothermal microwave assisted technique are performed.

Luisa Scolfaro
Texas State University

Date submitted: 11 Nov 2016 Electronic form version 1.4