Optical properties of ErH$_{2+x}$: First principles calculations and experimental measurements.$^{1}$ CLARK SNOW, THOMAS MATTSSON, Sandia National Laboratories — Rare earth and transition metal hydrides exhibit many interesting physical phenomena, from metal-semiconductor transitions to transparency changes at RT as a function of hydrogen content. Electrical resistivity measurements by P. Vajda (1) indicate that ErH$_{2+x}$ undergoes a metal-semiconductor transition between 240-290K and an antiferromagnetic transition between 1.75-2.3K depending on hydrogen content. These same transitions should also cause profound changes in the optical properties. This work will present first principles calculations of the optical properties of ErH$_{2+x}$ from 300-600K where x ranges from -0.2 to 0.2. The calculations will be compared to experimental results on thin films of ErH$_{2+x}$ which were obtained as a function of temperature from 10-600K and hydrogen content.

$^{1}$ Sandia is a multi-program laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy’s National Nuclear Security Administration under Contract DE-AC04-94AL85000.