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**Justin Droba\*** (drobajus@msu.edu). *Second Harmonic Generation at Metal/Dielectric Interfaces via Density Functional Theory*. Preliminary report.

Second harmonic generation (SHG), in which a material converts electromagnetic radiation at frequency  $\omega$  to that at  $2\omega$ , is perhaps the simplest yet most widely studied nonlinear optical phenomenon. Following the convention used for dielectrics, the nonlinear behavior is traditionally expressed mathematically by introduction of a polarization term  $\mathbf{P}^{\text{NL}}$  into Maxwell's equations. Bloembergen *et al.* derived a simple expression for  $\mathbf{P}^{\text{NL}}$  using the hydrodynamic model for electrons, but this model leaves much to be desired mathematically and physically. Thus, instead of using this classical model, we compute the electron density using density functional theory (DFT) and use that to calculate the current within macroscopic Maxwell Equations. In this presentation, I will present the basic theory of this approach as well as some preliminary results for 1D current in a 2D Maxwell system. (Received August 24, 2011)