1096-78-1621 **Justin Droba*** (drobajus@msu.edu), 6355 Beechfield Dr., Lansing, MI 48911. *A TD-DFT Approach to Second Harmonic Generation at Metal Surfaces.* Preliminary report.

Second harmonic generation is a simple nonlinear optical phenonemon in which a material converts incident light at frequency ω to that at 2ω. A classical model for the process at metal surfaces was developed by Nobel laureate Nicholaas Bloembergen using hydrodynamic equations. However, a multiphysics approach that combines modeling techniques from solid-state physics with linear response theory from time-dependent density functional theory (TD-DFT) provides a more appropriate framework to describe the process. The model's increased realism unfortunately is accompanied by a significantly involved chain of computations, each of which has its own challenges. In this talk, I will present the some of the basics of the TD-DFT modeling approach, provide a numerical example, and discuss some of the numerical techniques I used to demonstrate the example. (Received September 16, 2013)