Abstract Submitted
for the TSS18 Meeting of
The American Physical Society

Several Approaches to Realistic Dynamical Simulations in Advanced Materials MICHAEL TAGARAS, JIAN WENG, ROLAND ALLEN, Texas AM University — This talk will cover several methods for realistic dynamical simulations of advanced materials, including ultrafast phase transitions. In our first method, Ginzburg-Landau-like order parameters are coupled to one another and to the vector potential of an incoming laser pulse, so that the resulting phase transition is described by time-dependent Ginzburg-Landau theory. This approach is capable of describing one mechanism which is observed in light-induced superconductivity. Secondly, a new method will be introduced for treating ultrafast phase transitions, such as those involving superconductivity, magnetism, charge density waves, and spin density waves. Illustrative results will be presented for a toy model, with the electronic temperature immediately after the laser pulse calculated as a function of the fluence. Finally, we modify this approach with the addition of an electronic self-energy, which allows for calculations currently not possible with conventional density-functional-based methods.

Michael Tagaras
Texas A
M University

Date submitted: 08 Mar 2018 Electronic form version 1.4