Abstract Submitted
for the 4CF12 Meeting of
The American Physical Society

Neural Network Solutions to Optical Absorption Spectra CONRAD ROSENBROCK, Brigham Young University — Artificial neural networks have been effective in reducing computation time while achieving remarkable accuracy for a variety of difficult physics problems. Neural networks are trained iteratively by adjusting the size and shape of sums of non-linear functions by varying the function parameters to fit results for complex non-linear systems. For smaller structures, ab initio simulation methods can be used to determine absorption spectra under field perturbations. However, these methods are impractical for larger structures. Designing and training an artificial neural network with simulated data from time-dependent density functional theory may allow time-dependent perturbation effects to be calculated more efficiently. I investigate the design considerations and results of neural network implementations for calculating perturbation-coupled electron oscillations in small molecules.

Conrad Rosenbrock
Brigham Young University

Date submitted: 17 Sep 2012 Electronic form version 1.4