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## Title

Computational All-Electron Time-Dependent Density Functional Theory in Real Space and Real-Time: Applications to Molecules and Nanostructures

## Author

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## Degree Name

Doctor of Philosophy (PhD)

## Degree Program

Electrical and Computer Engineering

## First Advisor

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## Subject Categories

Electrical and Computer Engineering | Physics

## Abstract

Nowadays, for nanoelectronic devices, inter-atomic interactions and quantum effects are becoming increasingly important. For time dependent problem, such as high frequency electronics responses, or optical responses, the description of the system behaviour necessitates insights on the time dependent electron dynamics. In this dissertation, we proposed new effective modelling and numerical schemes to address the problem of time-dependent quantum simulations. An all-electron realspace real-time framework and TDDFT/ALDA type calculations are used for obtaining time dependent properties of molecules and nanostructures. Direct Hamiltonian diagonalizations are performed by using the innovative linear scaling eigenvalue solver FEAST. The spectral propagation schemes enable us to have much longer time steps, and it has been proven to be stable and highly scalable. A MPI parallel computing architecture is implemented, large monocles and nanostructures can be simulated in timely manner, which gives our model great advantage over traditional TDDFT calculation schemes. Optical absorption spectrum of small molecules are calculated and compared directly with the experimental values. Our results shows good agreement with experiments for a large selection of molecules. Finally, we apply our modelling and numerical schemes to study the (5,5) metallic Carbon Nanotubes, we successfully obtain the --and [arrow left] electrons plasmon which has been measured in experiments. Also, for the first time, we found the 1-D Luttinger liquid plasmon in 5 unit cell (5,5) CNT, whose plasmon velocity is consistent with other theoretical calculations.

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