# Finite Element Analysis of Molecular Rydberg States

M. G. Levy, X. Liang, R. M. Stratt, and P. M. Weber*
Brown University Department of Chemistry
*Corresponding author: Box H, 324 Brook Street, Providence RI 02912, Peter_Weber@brown.edu

## Introduction

In quantum mechanics there are very few analytically solved problems. One of the more famous ones is the Hydrogen Atom. In this study we liken more complicated molecules, like trimethylamine, to the hydrogen case, noting that these many-electron-containing molecules can be excited into a regime where the charge distribution of the molecular core can be approximated by a frozen charge density, leading to excited orbitals that resemble those of a Hydrogen Atom. Such highly excited states are known as Rydberg states. We calculate the electron binding energies associated with the Rydberg states of different molecules using quantum chemical *ab initio* calculations to compute the core charge distribution and compare our computational spectra with experimentally measured eigenvalues. We will also discuss aspects of using and importing the results from such calculations into COMSOL.

## Use of COMSOL

COMSOL is used in this study as a vehicle through which to solve the Schrödinger equation. We critically examine the effects of different meshes and solvers on the solution to a host of eigenvalue problems. The adaptive MATLAB interface of COMSOL allows us to import data from different chemistry calculator suites towards the end of solutions for very complicated eigenvalue problems. The coarse grained finite element approach yields good results, as this mesh based method handles the diffuse states better than more established basis-based chemistry suites (like Gaussian or Spartan), and enables us to verify both the orbital structures of the molecules and the eigenvalues.

## Expected Results

Here are some qualitative examples of computational results for certain Rydberg state wave functions.

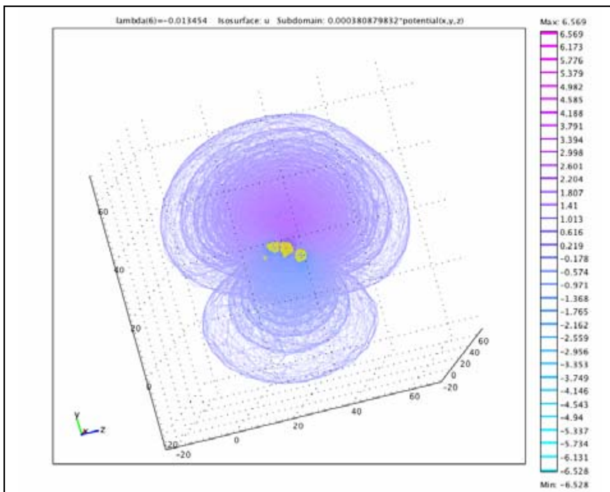


Figure 1. A 3p Rydberg State of Trimethylamine

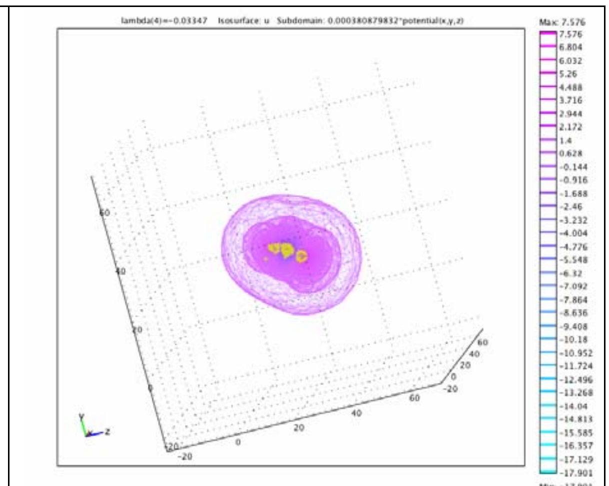


Figure 2. A 2s Rydberg State of Trimethylamine

We expect to fine tune our approach, achieving eigenvalues that are accurate into the 10 meV regime.

## Conclusion

COMSOL can be used as an effective tool to obtain computational eigenvalues for Rydberg state binding energies of molecules.