A Computational Approach to Studying the Properties of Photosensitizers in Photodynamic Therapy

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What is photodynamic therapy?

• Photodynamic therapy (PDT): Type of treatment which uses a photosensitizer, light, and oxygen to destroy nearby cancer cells.
What are photosensitizers?

• Photosensitizer: Molecule which produces a chemical change in other molecules via a photochemical process (i.e. excitation by light)

• We focus on studying boron dipyrromethene (BODIPY) dyes and their specific application to PDT

• BODIPY dyes: Fluorescent compounds used in
  • Biological imaging
  • Solar cells
  • PDT
Studying chemistry via the computer

• Computational Chemistry
  Solving the Schrödinger equation
  (equation used to calculate energy based on electronic wavefunction)

\[ \hat{H}\Psi = E\Psi \]

• Computable: $E_{GS}$, $E_{ex}$, $E_{em}$, couplings, vibrational frequencies, charge density, and more

• Accelerates normally extensive processes:
  • Selecting, synthesizing, and testing candidate compounds
  • Measuring properties
Outline of thesis work

• Compute photophysical properties of a set of BODIPY dyes
• Verify methods in use
• Study the interaction of oxygen with a BODIPY dye
• Investigate the $^{1}\text{O}_2$ generation properties of a BODIPY dye
Computational methods

• **Density functional Theory (DFT):** Method to calculate electronic ground states
• **Time-Dependent density functional theory (TD-DFT):** Method to calculate electronic excited states
• **Restricted open-shell Kohn-Sham (ROKS) method:** Method to calculate electronic excited states
• **Constrained density functional theory (CDFT):** Method to constrain atoms/molecules to obtain specific electronic states \(^1\text{O}_2, \, ^3\text{O}_2, \, \text{etc.}\)
Computing photophysical properties and verifying ROKS
Interaction of $O_2$ with BODIPY
Interaction of O$_2$ with BODIPY
Investigating $^{1}\text{O}_2$ generation

- Compute couplings between electronic states
- Solve for rate of $^{1}\text{O}_2$
Conclusions, future work and applications

• Verified use of ROKS as a viable excited state method
• Characterizing the $^1\text{O}_2$ generation characteristics of a BODIPY chromophore
• Setting foundational work for future scientist working with chromophores used in PDT
• Create a protocol to quickly sort through large sets of candidate dyes to find which have the best properties for use as photosensitizers in PDT
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Questions?