Ariel Gale

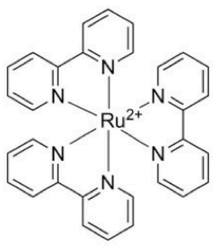
Ph.D. Student, Chemistry
Third Year ARCS Scholar
Jeanne Berry Award

EMORY UNIVERSITY

Optimizing methods to design photoredox catalysts

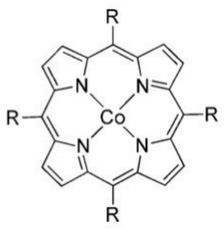
The design and discovery of photoredox catalysts is accelerated by computational prediction of key properties. Optimizing the methods used to simulate molecules can improve the accuracy without increasing the cost of a calculation.

Transition Metal Complexes



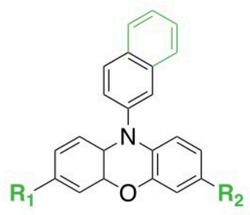
- Expensive and rare metals
- Most researched

Porphyrins



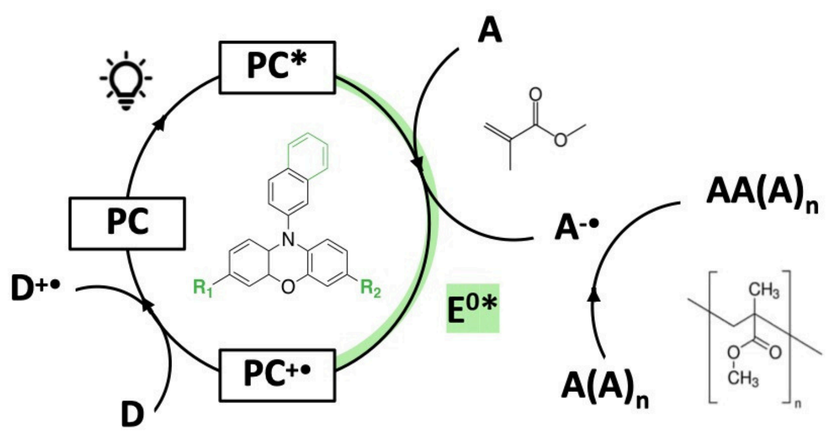
- More common metals
- Biology-inspired

Organics

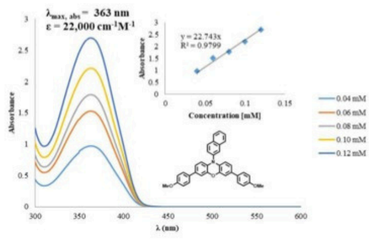


- Metal free
- Diversity of potential catalysts

Photoredox Catalyst Cycle



Experimental methods

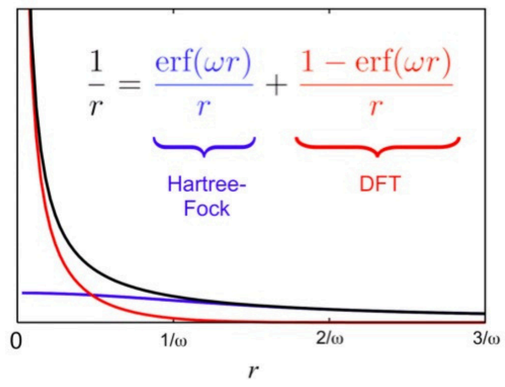


- Synthesis and analysis for each molecule
- Unique materials and methods

Computational methods

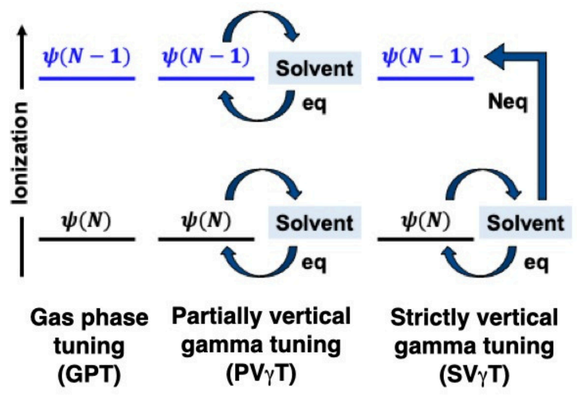
- Choose accuracy vs. speed for application
- Use same method for all molecules

Range-separated hybrid functionals



- Electron exchange split into short range (SR) and long range (LR)
- Hartree-Fock in the long range is useful for charge transfers
- ω separates SR and LR

Optimal ω Tuning Schemes



	Lit.	Me
GPT		0.6 V
PVγT		0.3 V
SVγT		0.9 V

Explanation: Density Delocalization

PVγT has less error because it is more linear than SVγT

I would like to acknowledge my advisor, Dr. Fang Liu, the Liu lab for helpful discussions, and the Emory University Department of Chemistry and the National Science Foundation for their financial support.

Scholar Awards Celebration
November 15, 2023

SCHOLAR AWARDS CELEBRATION · ARCS · ARCS FOUNDATION ATLANTA

Igniting Innovation in Georgia