Ariel Gale

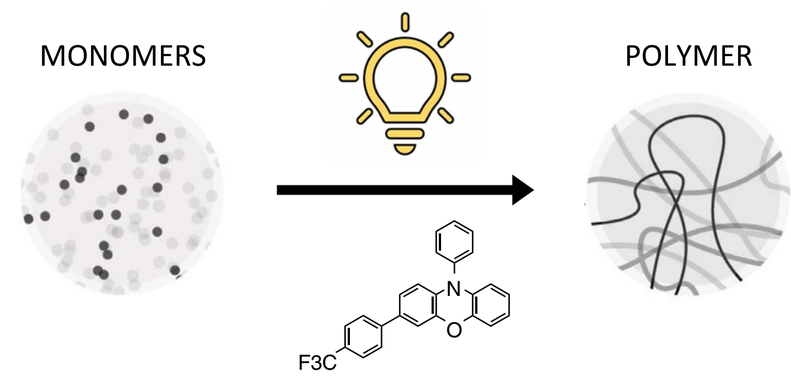
Ph.D. Student, Chemistry
Second Year ARCS Scholar
Hawkins/ARCS Award

EMORY UNIVERSITY

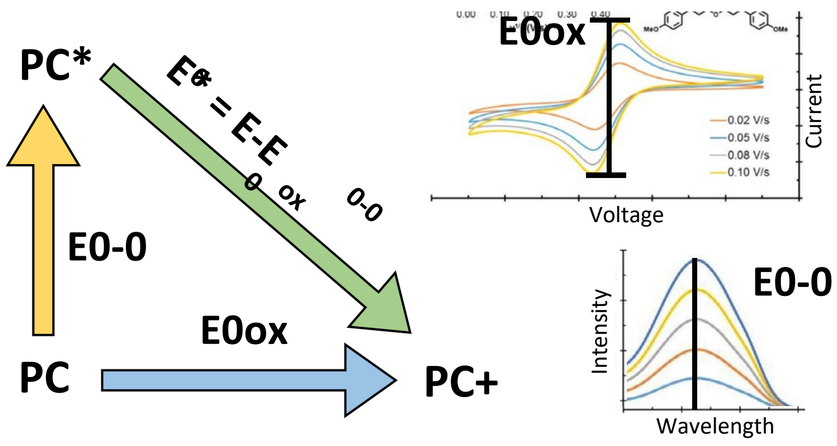
Optimizing Methods to Design Photoredox Catalysts

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.

PHOTO	REDOX	CATALYSIS
Light changes the **energy** of electrons	Energy changes the **location** of electron	Molecule changes the **speed** of reaction

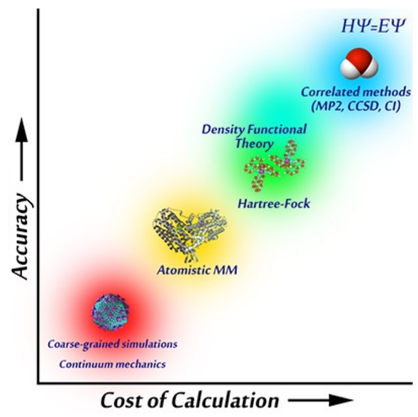


The catalyst allows the monomers to link together under visible light and form a polymer.

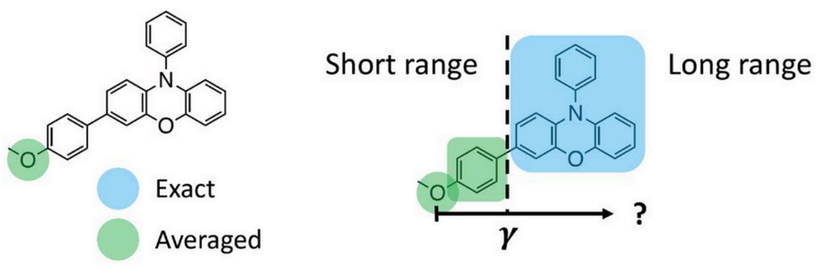


Computer simulations can replace chemistry experiments!

How accurate are they?

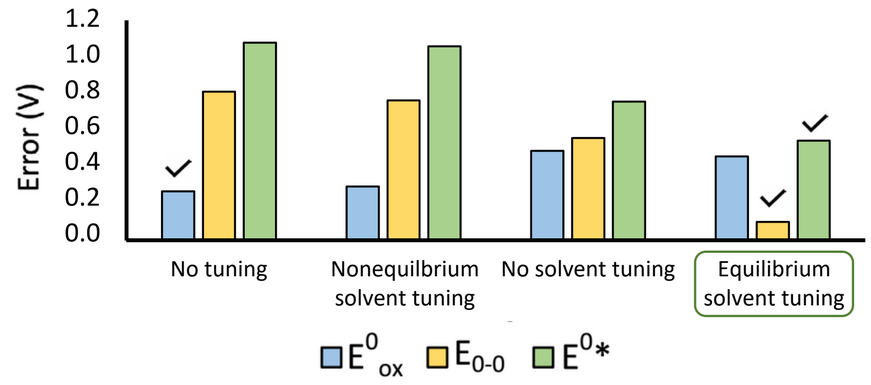


Density **F**unctional **T**heory is a popular low-cost option that uses quantum mechanics to simulate chemistry.



I test procedures that can **improve the accuracy** of DFT without increasing the cost by **tuning** parameters.

Tuning procedures improve accuracy for light-driven properties but not for redox properties.



Footnotes: J. Am. Chem. Soc. 2018, 140, 15, 5088–5101.
https://leeping.github.io/forcebalance/doc/html/index.html.

ARCS FOCUS ON THE FUTURE 2022

Scholar Awards Celebration
November 17, 2022