



QuEST: Quantum Electrodynamics for Selective Transformations Center for Chemical Innovation

Grant CHE-2124398 PI: Todd D. Krauss, University of Rochester



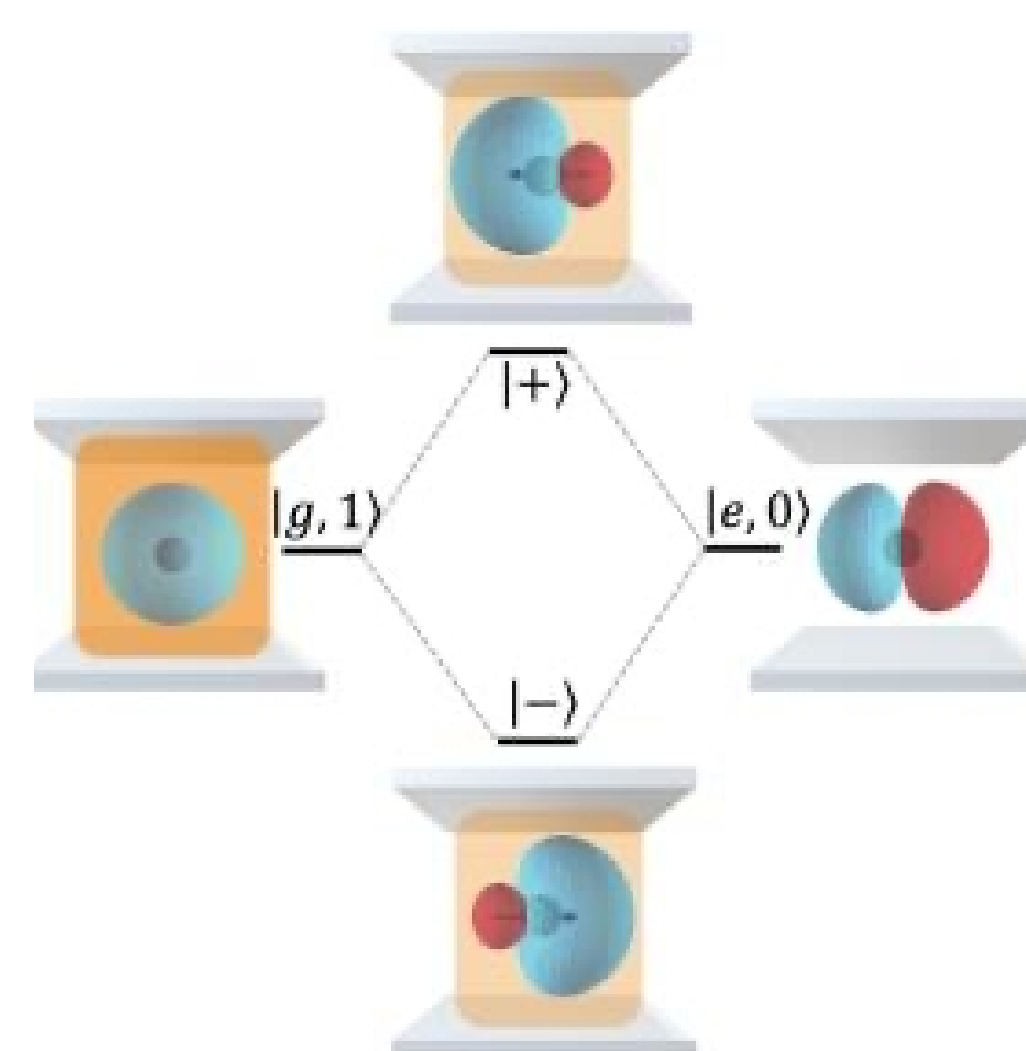
The goal of QuEST is to *change chemical reactivities* using molecular polaritons.

Can the reactivity of molecules be altered by changing their molecular orbitals through strong light-matter coupling?

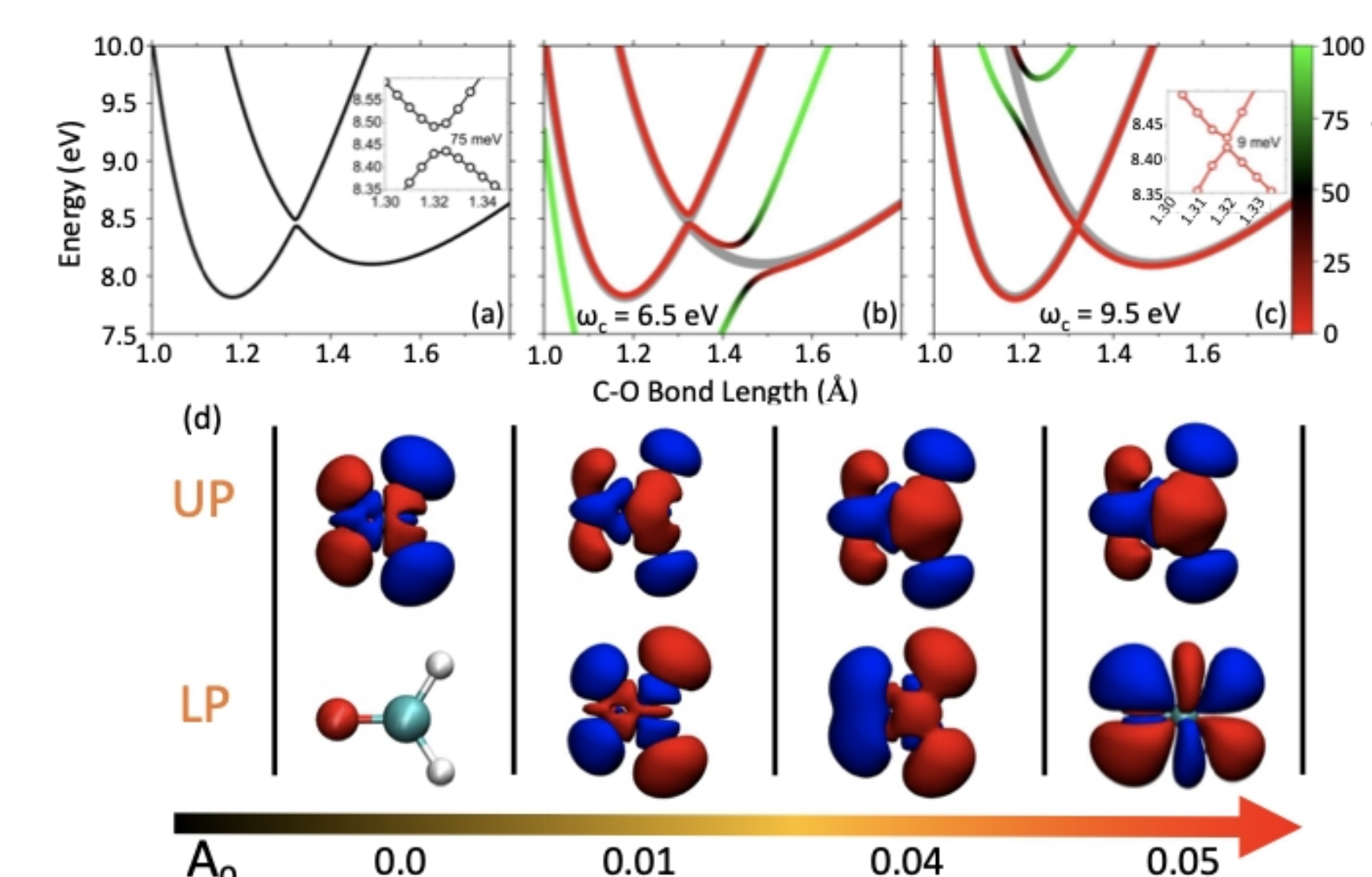
- A **grand challenge** in chemistry is to exhibit **selectivity and control** over a chemical transformation
- Established rules** of reactivity fundamentally depend on the **interaction of molecular orbitals**
- To **change these rules**, we will change molecular orbitals through **coupling molecules to an optical cavity**

Electron Polariton: quasiparticle formed by hybridizing electronic states of molecules with the quantum-radiation field of an optical cavity

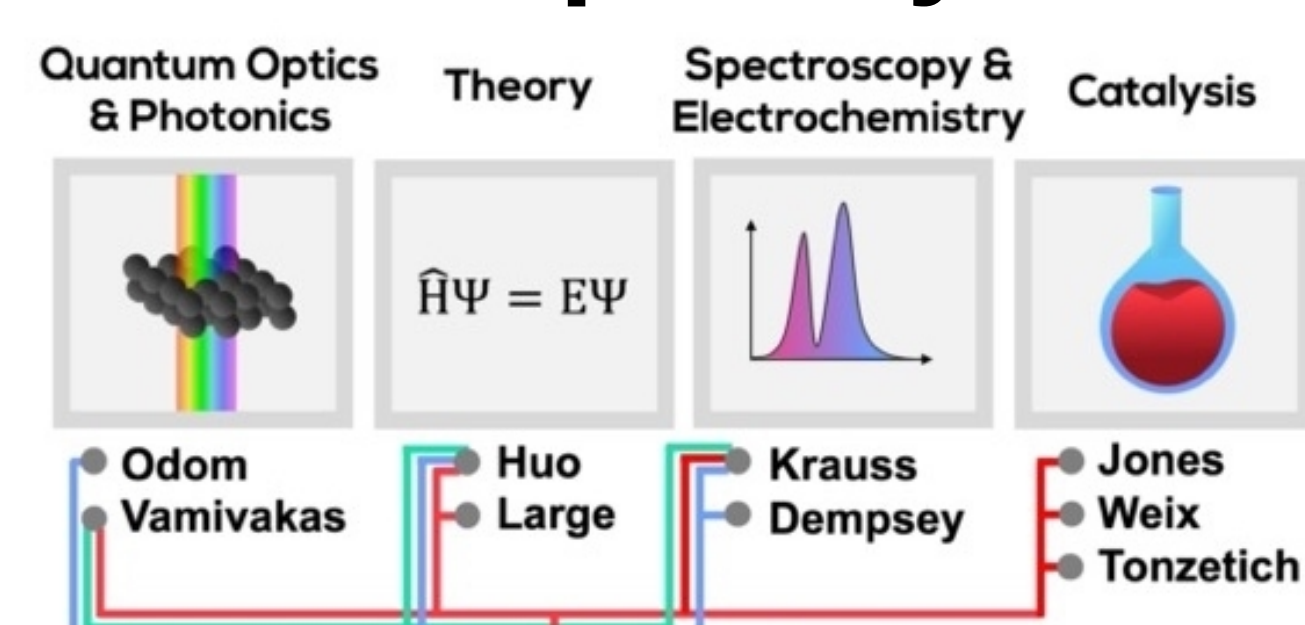
- Polaritons result in a superposition of **excited and ground states** creating **new molecular orbitals**



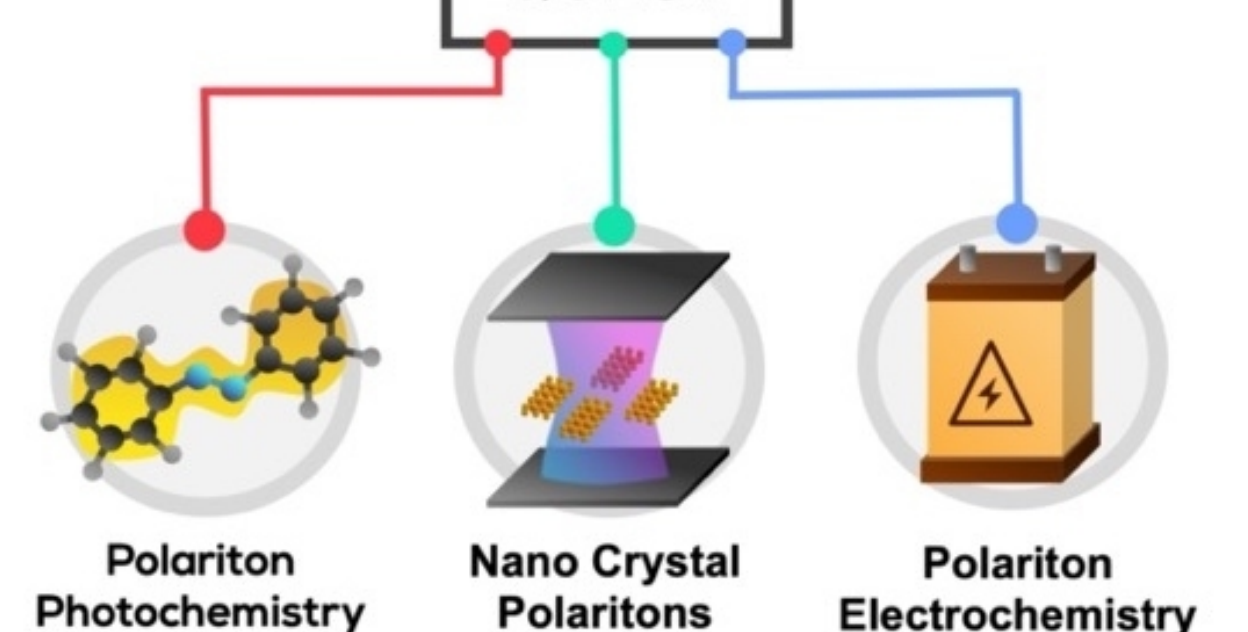
- Polaritons can offer a **new tool for chemists** to change the pathway of a reaction, similar to chemical catalysts
- Tune** reaction outcomes with properties of **light**



Multidisciplinary Team



QUEST



University of Rochester

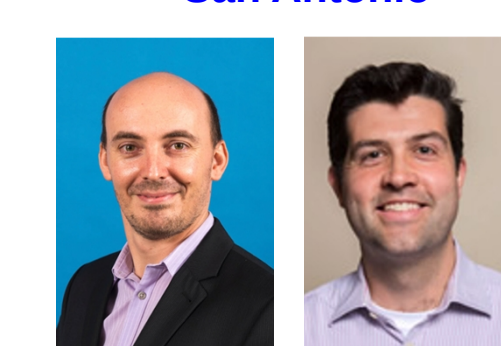
University of North Carolina at Chapel Hill

Northwestern University

University of Wisconsin-Madison



University of Texas, San Antonio



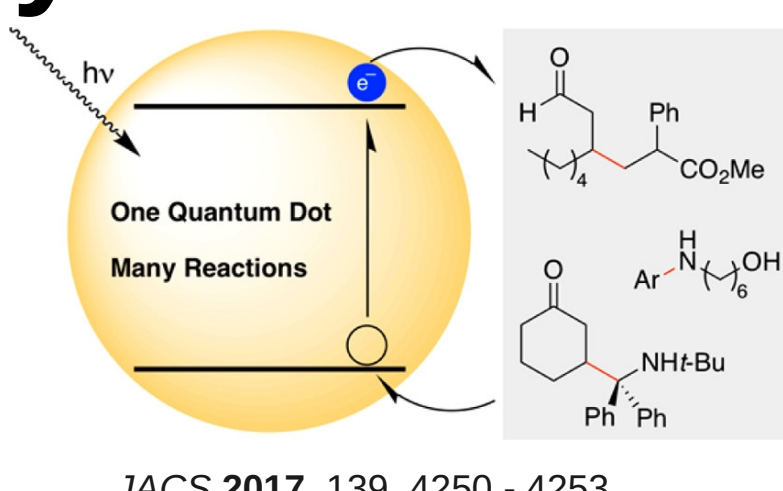
The University of Texas at San Antonio



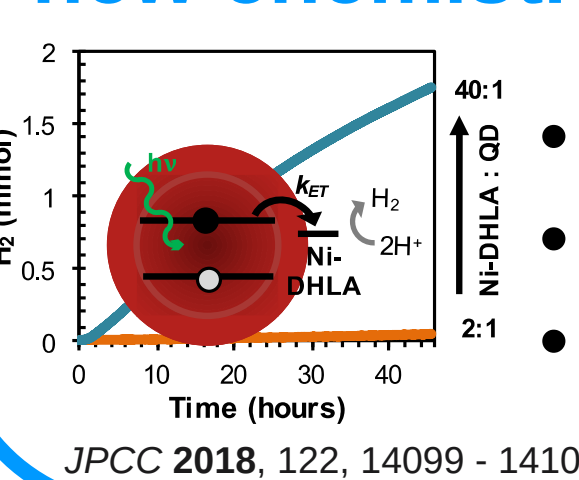
Sustainability Initiative

Using (sun)light and nanocrystals inside an optical cavity to **unlock new chemistries** for:

- Sustainable fuel forming reactions
- Photoredox Catalysis
- Greener chemical syntheses



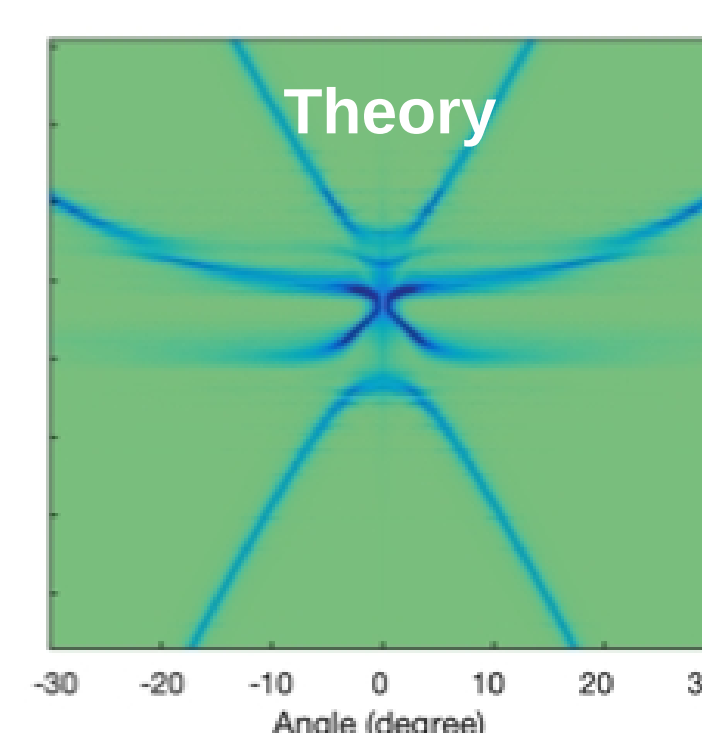
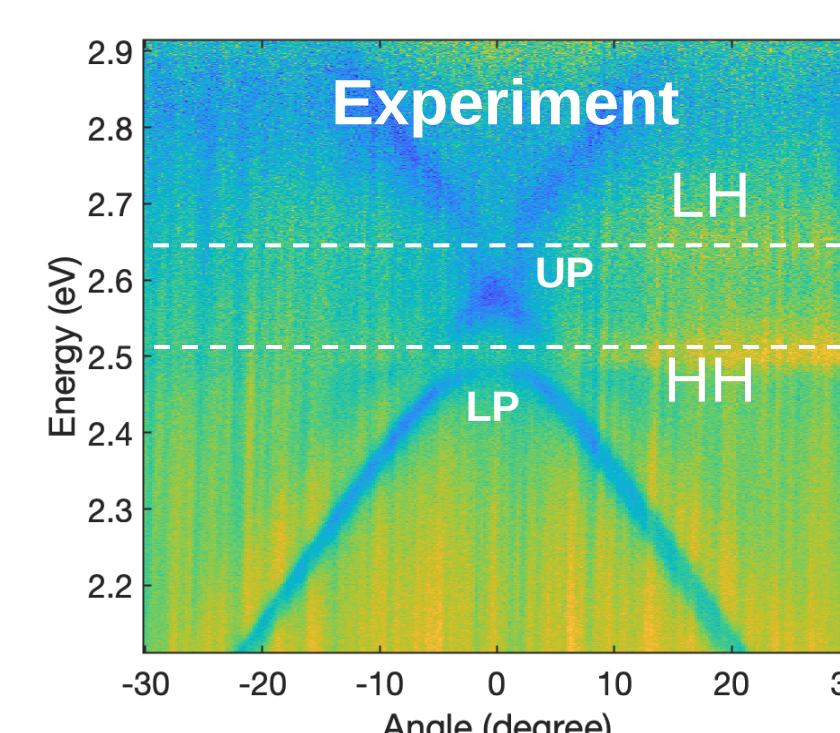
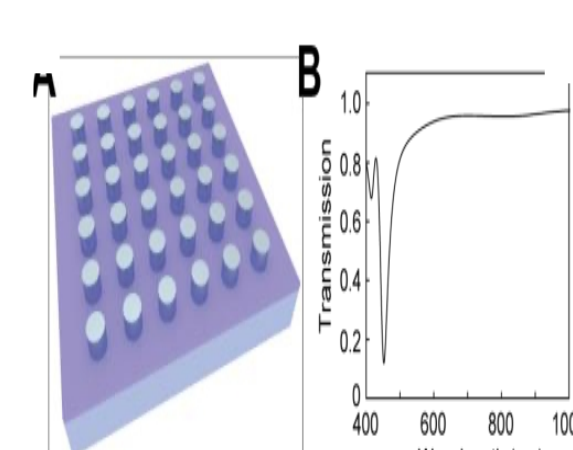
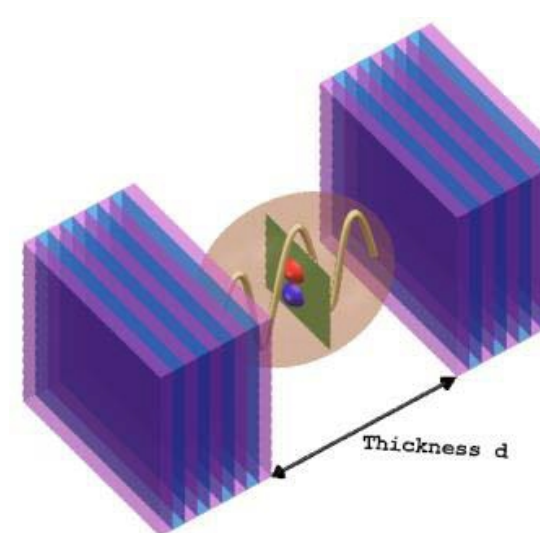
JACS 2017, 139, 4250 - 4253



JPC 2018, 122, 14099 - 14106

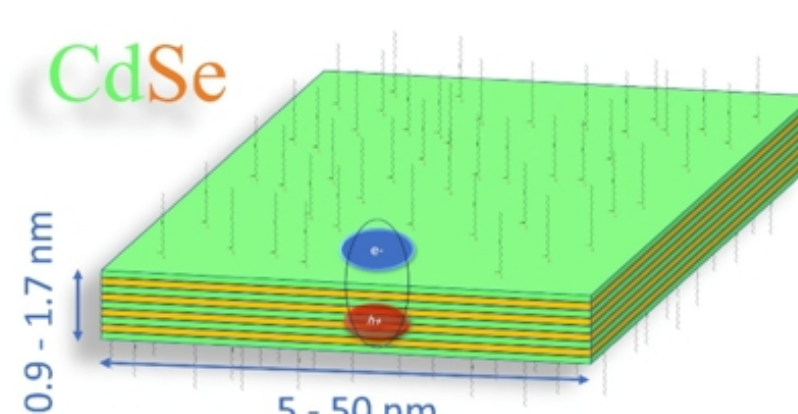
Couple Nanocrystals to Optical Cavities

Dielectric Optical Cavity

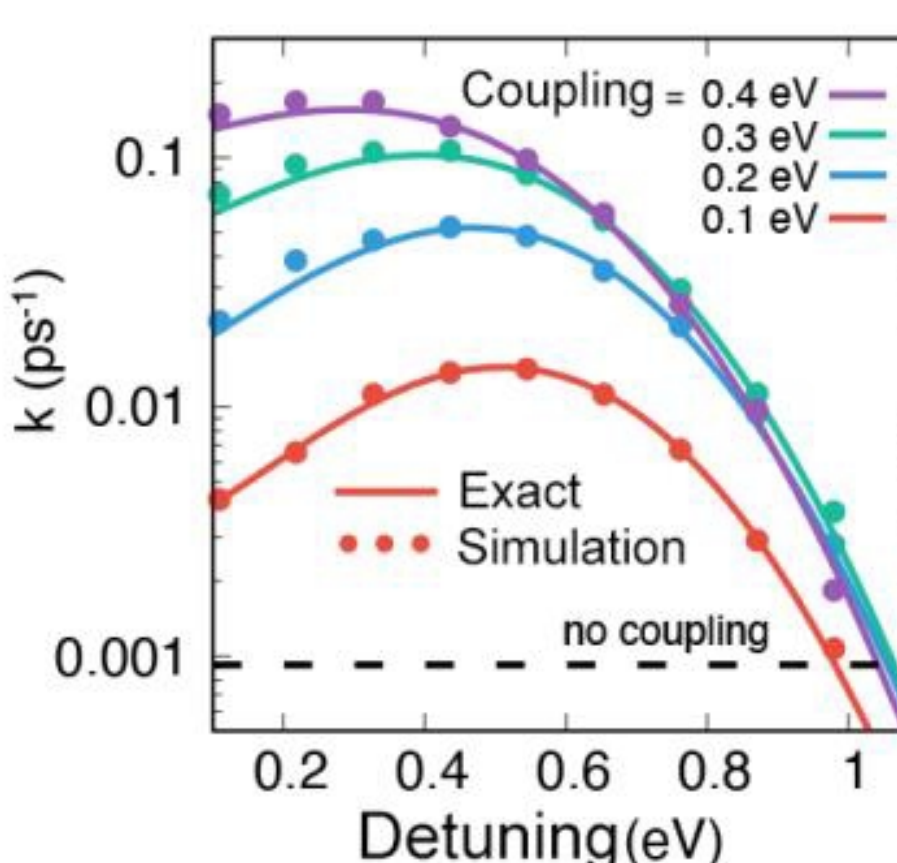


Lattice Plasmon Array

2D Nanocrystals



- Large oscillator strength
- 2D transition dipole in plane
- Narrow fluorescence spectra

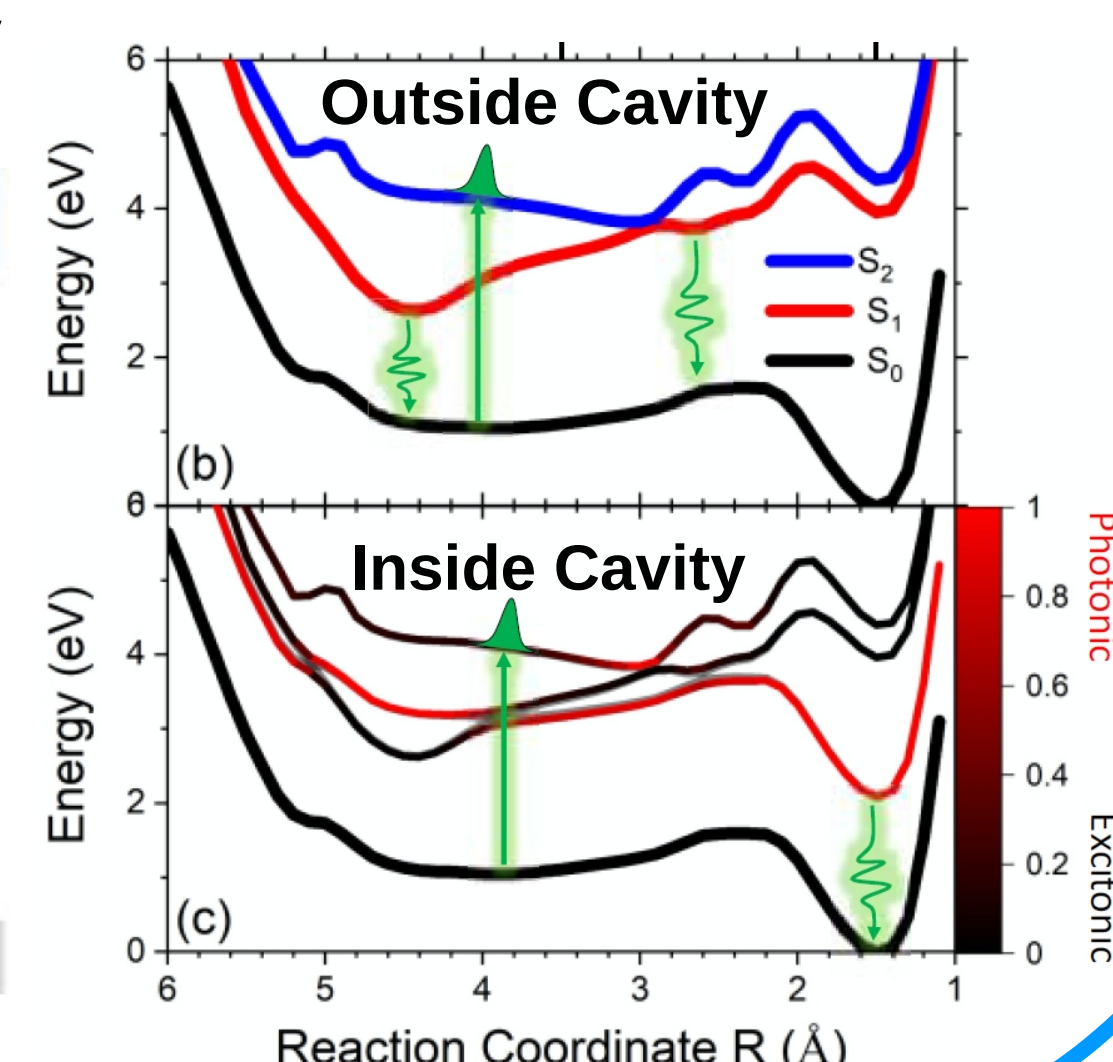
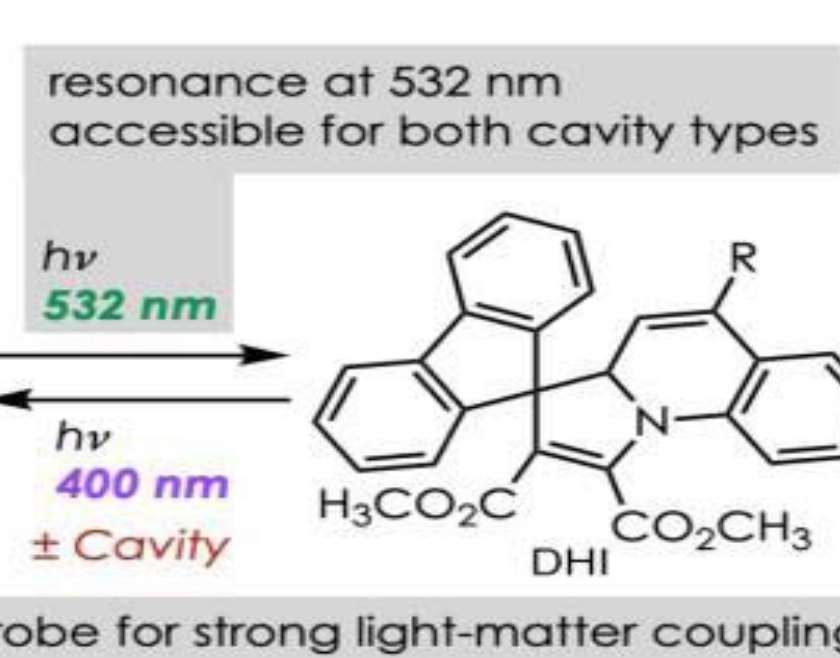
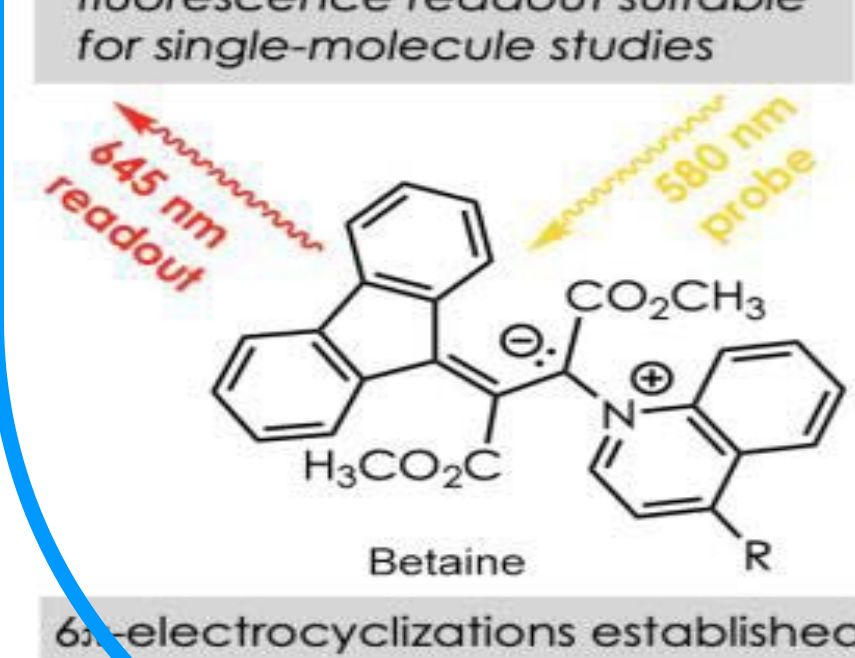


Modify Electron Transfer Rates

Polariton Mediated Reactivity

Single-Molecule Studies of Cavity

fluorescence readout suitable for single-molecule studies



Broader Impacts

Education and Professional Development

Training in:

- Mentorship
- Science communication
- Science writing for general and expert audiences

Broadening Participation

- QuEST-specific REU program
- Address STEM "leaky pipeline" for URM students

Outreach and Informal Science Communication

- Educate Public about Quantum Science
- Collaborate with local science centers
- Community events
- Social media



QUEST Winter Conference



UTSA undergraduate honored with Outstanding Research Award for QuEST research



Outstanding College of Sciences Undergraduate Student



Outreach at local market



Acknowledgements

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<https://www.rochester.edu/question/>

