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Fifth Annual CMQT Symposium

April 23 & 24, 2026 | Northwestern University

Claudia Avalos

Claudia Avalos is an experimental physical chemist with a penchant for theory. Her research interests include solid-state nuclear magnetic resonance (NMR) spectroscopy, electron paramagnetic resonance (EPR) spectroscopy and nitrogen-vacancy (NV) center magnetometry development and application. After obtaining her B.S in Chemistry at the California State University Chico, she obtained her PhD at the University of California Berkeley. While at UC Berkeley, she investigated spin coupling interactions between defect NV centers in diamond and explored the use of these systems for sensitive magnetic field sensing and NMR signal enhancement applications. During her postdoctoral work at the École Polytechnique Fédérale de Lausanne she developed dynamic nuclear polarization methods for improving the NMR detection sensitivity for ^{19}F nuclei and investigated structural phase transitions in perovskite ferroelectric materials using solid-state magic angle spinning NMR. While in Lausanne, she also investigated optically induced spin polarization transfer in a number of novel pentacene-radical compounds using transient EPR. Now at NYU, Prof. Avalos is interested in pursuing research focused on using optical and magnetic resonance spectroscopies to better understand the spin physics, structure and function of photoactive materials such as ferroelectrics, perovskites and organic chromophores.

B.S. in Chemistry and Biochemistry at California State University Chico
PhD in Physical Chemistry at UC Berkeley with Alex Pines on "Detection and polarization of electron and nuclear spins in diamond"

Postdoc: Ecole Polytechnique Federale de Lausanne with Lyndon Emsley, worked on "Dynamic nuclear polarization and characterization of ferroelectrics"

Awards: Teaching Innovation Award, NSF CAREER, ACS PRF

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Predicting J-mediated Enhanced Intersystem Crossing in Chromophore-Radical Systems

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Chromophore-radical (C-R) systems have attracted attention in the spin physics community as potential candidates for dynamic nuclear polarization and quantum sensing due to their favorable optical and spin properties.[1] Similar to the NV^- center in diamond, the photoexcitation and subsequent relaxation of a C-R system may lead to a non-Boltzmann ground state spin polarization.[2] The magnitude of the triplet/radical exchange parameter J_{TR} has been predicted to vary by orders of magnitude from fractions to hundreds of cm^{-1} in a pentacene based organic C-R systems, and is directly related to the degree of conjugation between the chromophore and radical electrons.[3] A wide range of J_{TR} values and different coupling regimes are possible, and the ability to reliably predict the particular photophysics a C-R system is likely to exhibit based on ab initio excited-state coupling calculations would be highly beneficial for informed molecular design.

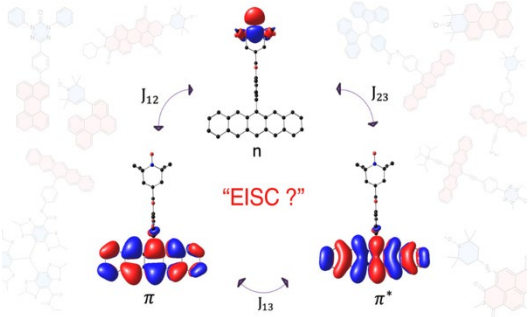

Figure 1. J-mediated enhanced intersystem crossing in pentacene-radicals.

In this work, we performed CASSCF/QD-NEVPT2 calculations to obtain the correct electronic wavefunctions and energies of electronic states in C-R systems. Using these results, we applied first-order perturbation theory to calculate a mixing term, κ, between the excited sing-doublet (SD_2) and trip-doublet (TD_1) states. Subsequently we compared these results to our own experimental datasets as well as those available in the literature which identify the presence or absence of J-mediated enhanced intersystem crossing. We then identify a threshold value of κ above which we expect to observe J-mediated EISC and design three candidate structures that we expect to exhibit spin polarization at specific magnetic field conditions. This work paves the way towards clear and effective tools for predicting the optical spin pathways of this class of molecular spin systems.

[1] Quintes, T.; Mayländer, M.; Richert, S. Nature Reviews Chemistry 2023, 7, 75–90.
[2] Avalos, C. E.; Richert, S.; Socie, E.; Karthikeyan, G.; Casano, G.; Stevanato, G.; Kubicki, D. J.; Moser, J. E.; Timmel, C. R.; Lelli, M., et al. The Journal of Physical Chemistry A 2020, 124, 6068–6075.
[3] Weiss, P. S.; Paz, A. S.; Avalos, C. E. Phys. Chem. Chem. Phys. 2025, 27, 8052–8076.