2021 Virtual HBCU-UP/CREST PI-PD Meeting

# Quantum-Mechanical Investigation of Structure-Property Relationships in Organic Emitters for Efficient Thermally Activated Delayed Fluorescence (TADF)

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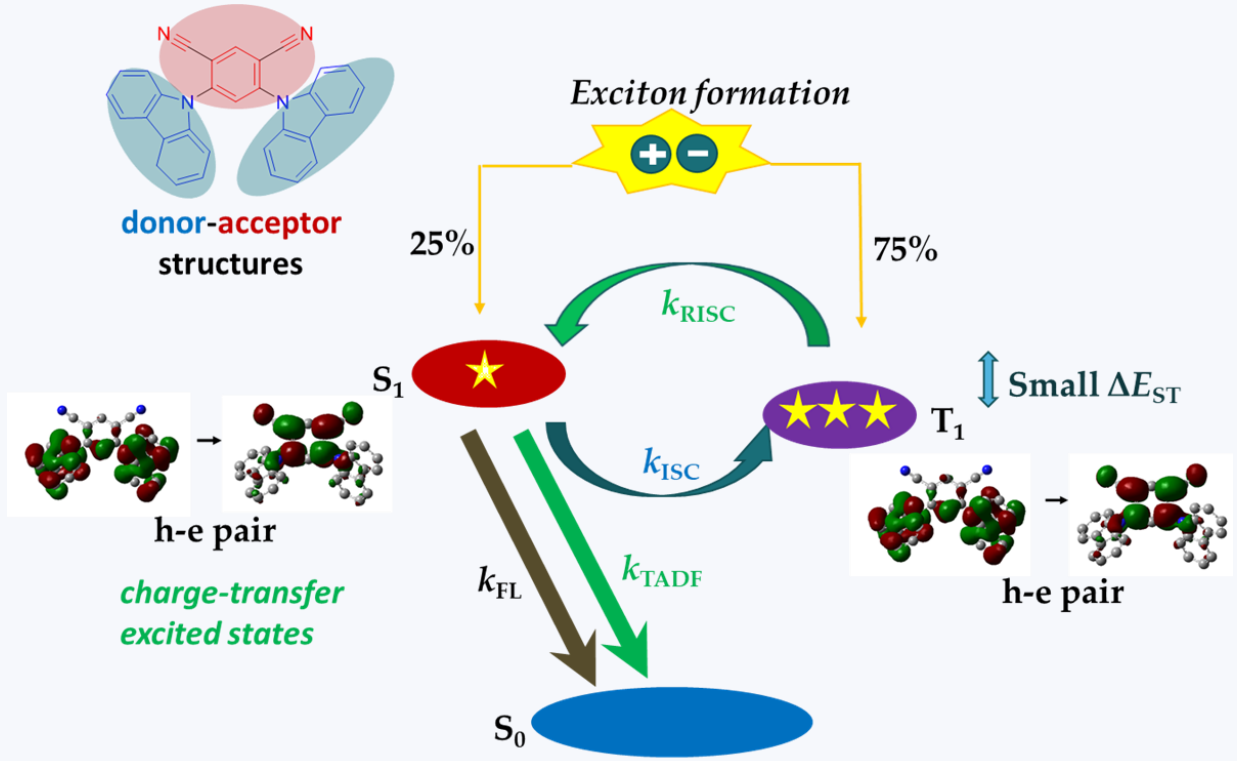
All findings and opinions are those of the authors, not necessarily of the funding agency or AAAS.

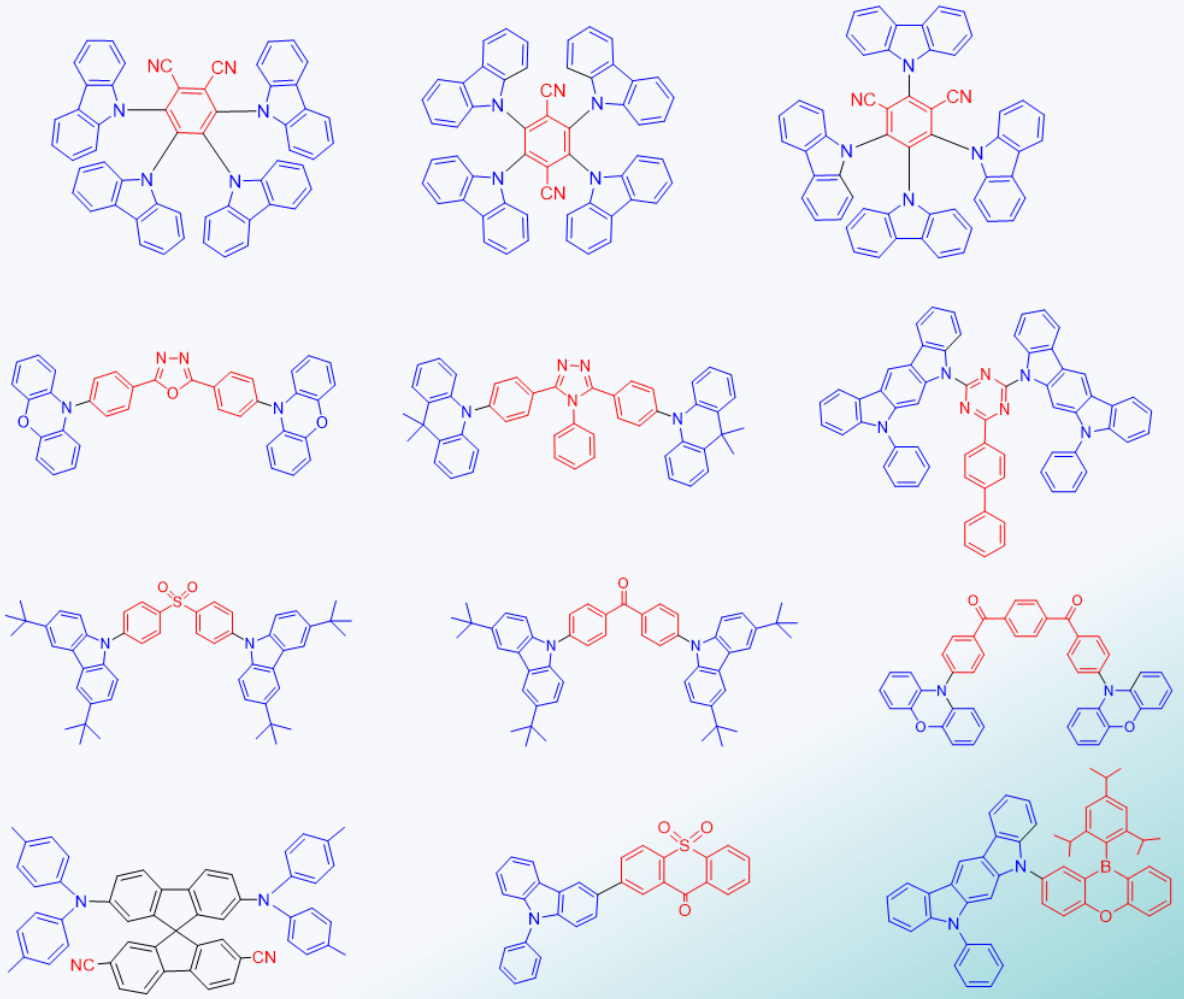
# Project Overview




- Theoretical characterization of the photophysical properties in donor-acceptor-type molecules that show Thermally Activated Delayed Fluorescence by using Density Functional Theory methods.
- Quantum-mechanical calculations of ground and excited-state geometries, energies and characterization of the nature (contributions from charge-transfer and localized-excitations) of the excited states via Natural Transition Orbital analyses.

# Best Practices/Successes

- The general strategy to maximizes the conversion of triplets into singlets (RISC) is to minimize the spatial overlap between the HOMO and LUMO frontier orbitals that minimizes the exchange energy and brings the singlet and triplet excited states close together (small $\Delta E_{ST}$).
- This is usually achieved in D-A compounds where the HOMO (LUMO) is primarily localized on the D (A) moiety.



# Implications

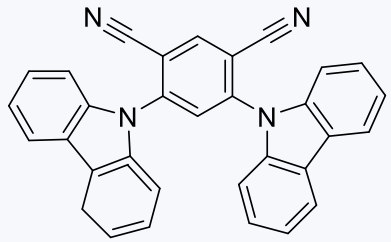
- As a consequence of this large spatial separation, the lowest singlet and triplet excitations usually feature a strong intramolecular CT character, which is not always compatible with intense emission requirements (high oscillator strength and large transition dipole moment).

- The choice of the donor and the acceptor appears to be very crucial since in some instances, a Locally Excited triplet state ($^3$LE) localized either on the donor or the acceptor becomes more stable than the CT states, thus hindering the triplet to singlet interconversion and leading to inefficient TADF.

# Identified Gap(s) for Future Collaboration or Enhancement

## Preliminary calculations

- The lowest singlet and triplet excited state energies were calculated by using TD-DFT based on the Tamm-Dancoff Approximation (TDA) on the optimized ground state geometries by using OT-SRSH approach combined with PCM.




DCzIPN

Known blue emitter selected for benchmark calculations

Cho, Y. J., Yook, K. S., Lee, J. Y., Sci. Rep., 5:7859, 2015

## Future Collaboration / Enhancement

- New sets of molecules – Collaborations with organic chemists
- Photoluminescence experiments – new mechanisms for light emission
- What we can do computationally?
- Characterize GS and ES geometries and energies, nature of ES, SOC effects, MD studies.
- Develop structure-photophysical relationships for new molecules.