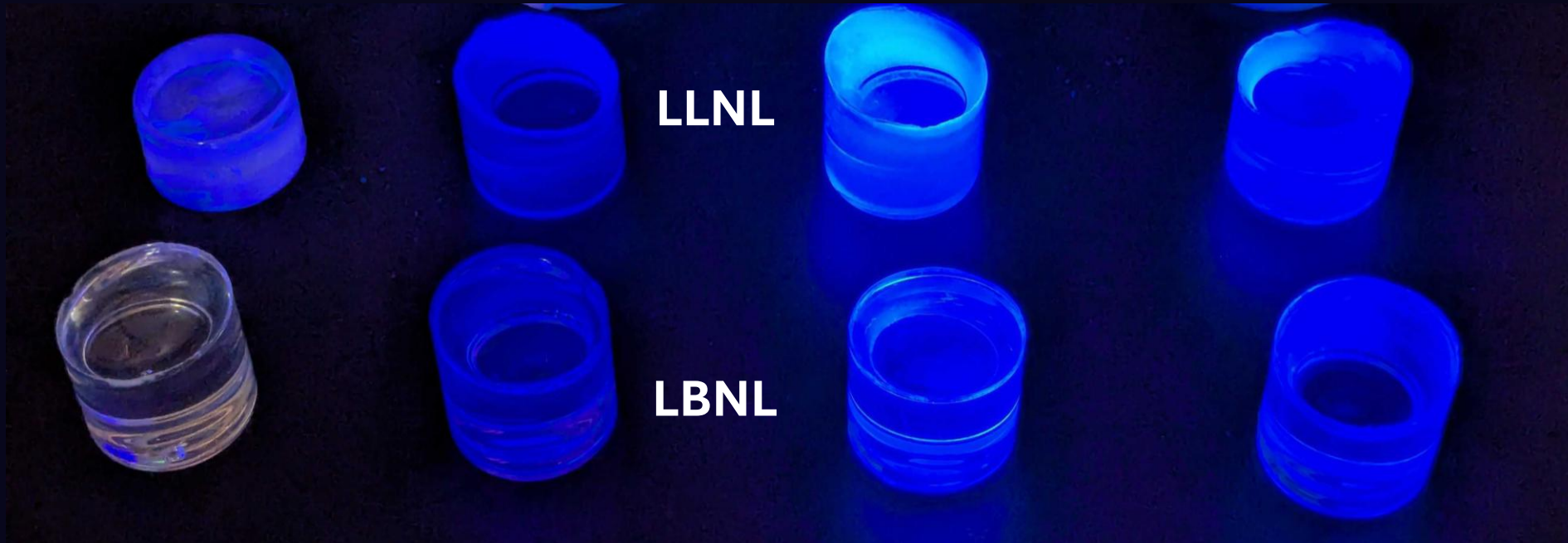


Investigating the Energy Transfer Mechanisms in Polystyrene based Plastic Scintillators



Dallar Babaian



Weronika W. Wolszczak (PI)
Scintillation Mechanisms



Vassilia Zorba
Laser Spectroscopy



Federico Moretti
Materials Sciences

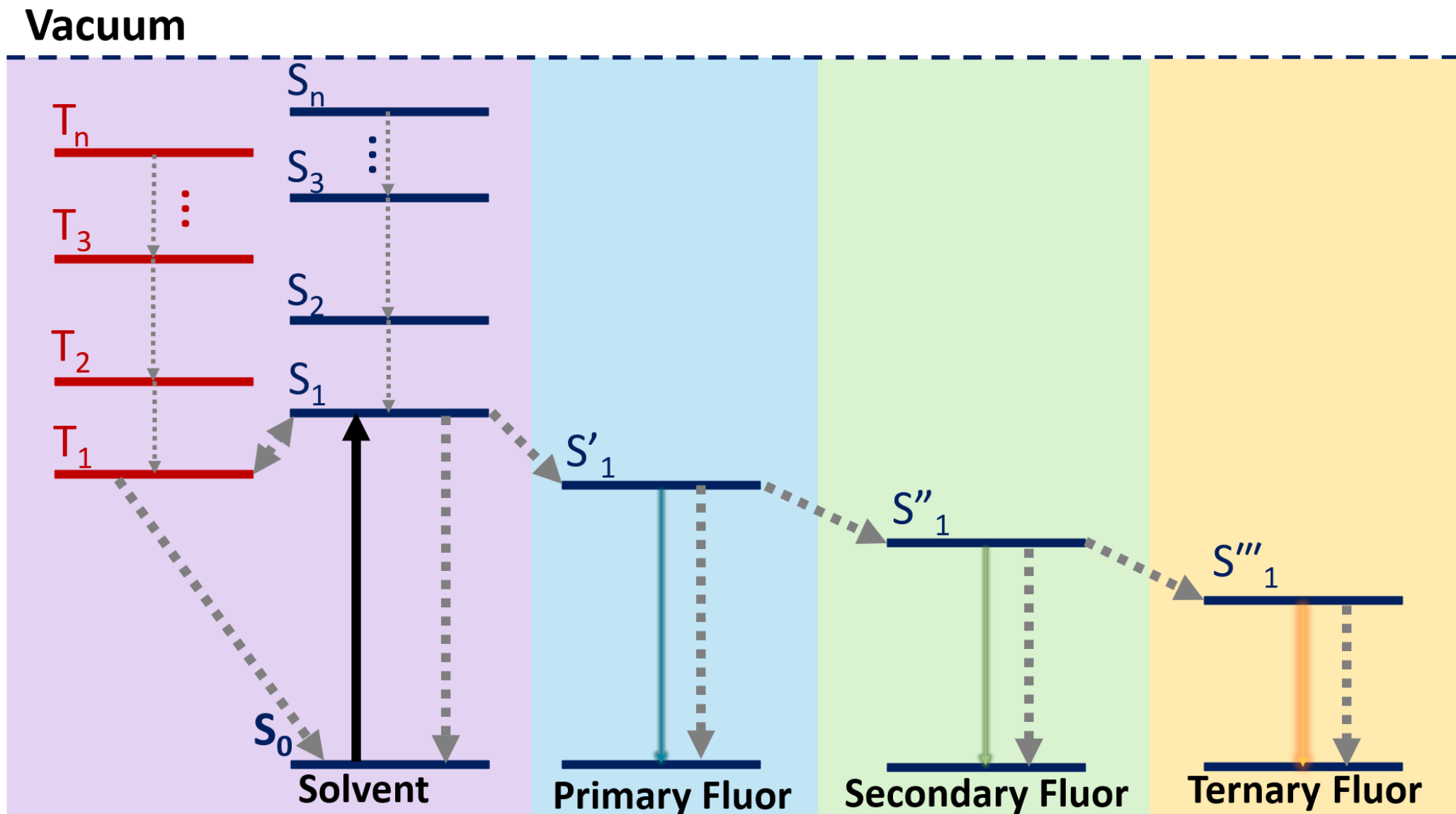


Dallar Babaian
Postdoctoral Fellow
Ultrafast Laser
Spectroscopy



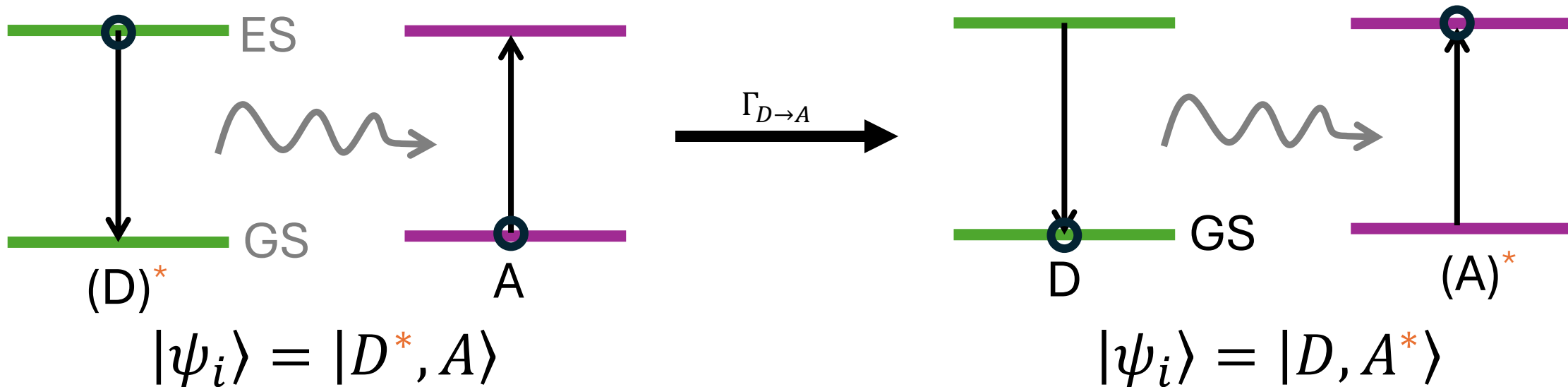
Ana Barrera-Jauregui
NNSA-IMPACT Intern
Chemistry

Current understanding of the scintillation mechanism



Resonant Energy Transfer

Fermi's Golden Rule:
$$\Gamma_{i \rightarrow f} = \frac{2\pi}{\hbar} |\langle \psi_f | V | \psi_i \rangle|^2 \delta(E_f - E_i)$$

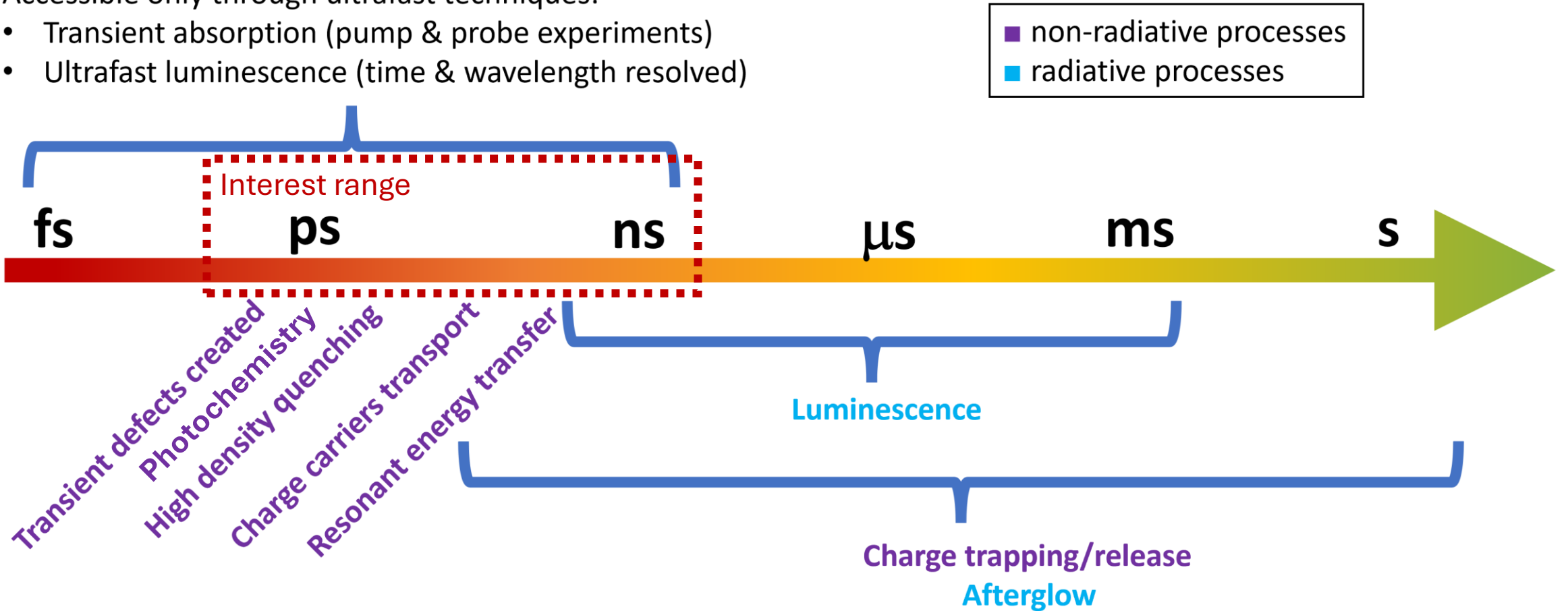


$$\Gamma_{D \rightarrow A} = \frac{1}{\tau_D} \frac{9(\ln 10)\kappa^2}{128\pi^5 n^4 R^6} \int F_D(\lambda) \varepsilon(\lambda) \lambda^4 d\lambda$$

Donor decay time Donor-Acceptor distance Normalized donor emission Acceptor molar extinction coefficient

Accessible only through ultrafast techniques:

- Transient absorption (pump & probe experiments)
- Ultrafast luminescence (time & wavelength resolved)



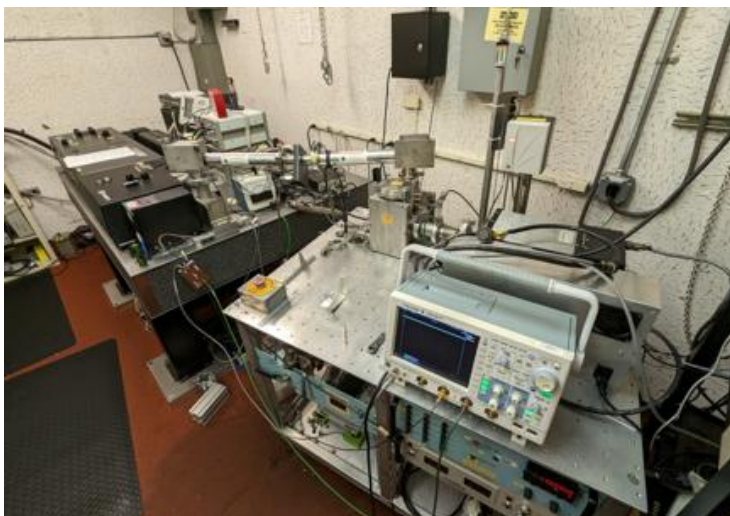
Steady State and Time Resolved Photoluminescence



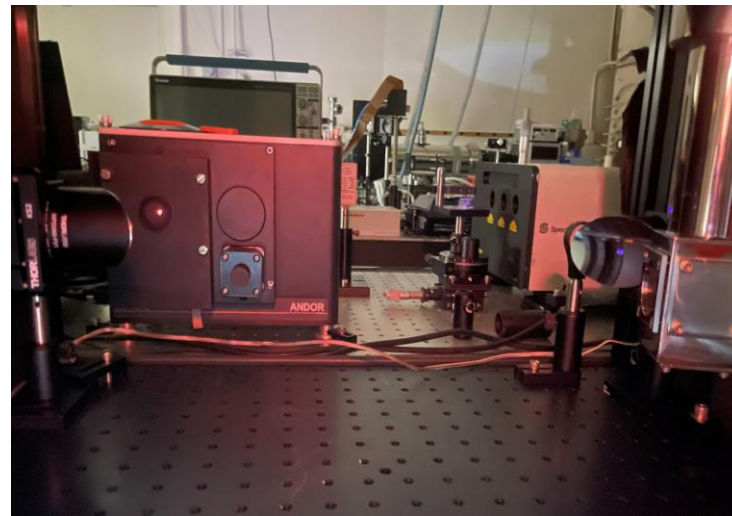
Radioluminescence



Pulsed X-Ray



Pulsed Photoluminescence



Studying Deconstructed Scintillators

Disassembling Scintillation Mechanisms



Polystyrene



Polystyrene + PPO



Polystyrene + bis-MSB



Polystyrene + PPO + bis-MSB

Study Building Blocks



Polystyrene



PPO

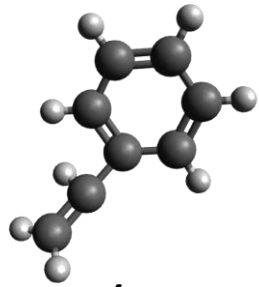
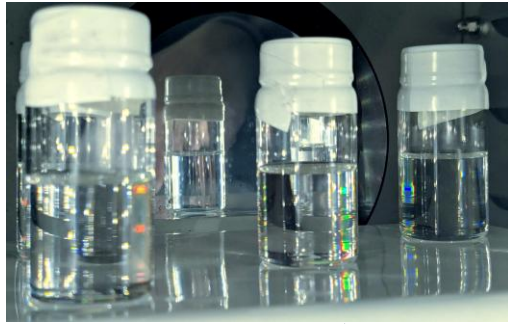


bis-MSB

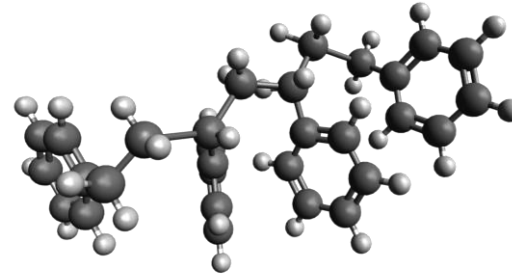
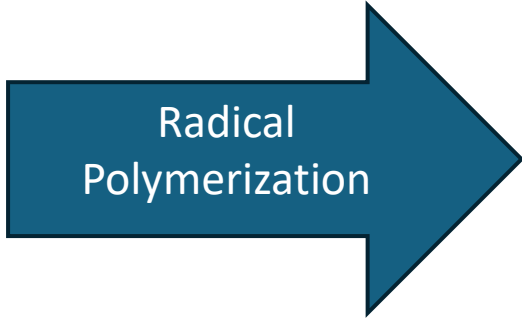
Combine & Rebuild



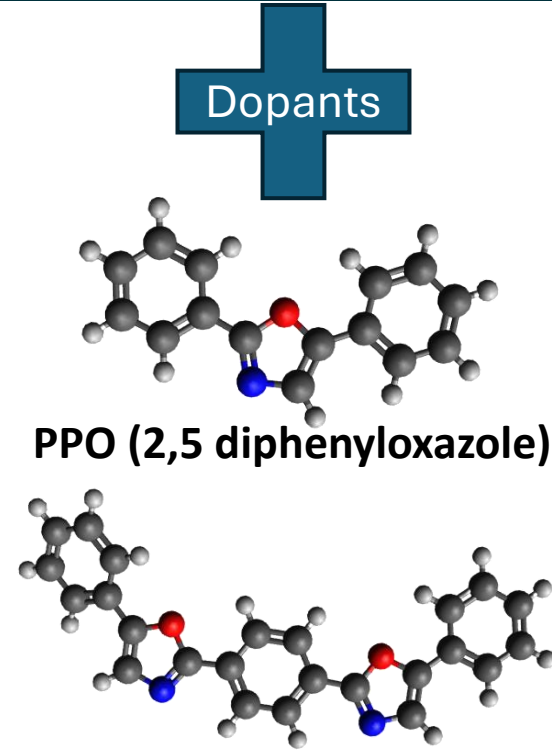
Sample Synthesis



Styrene (monomer)

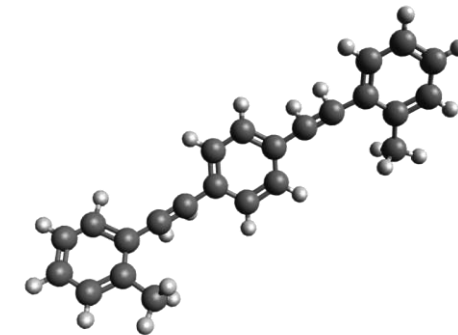


Atactic Polystyrene



PPO (2,5 diphenyloxazole)

POPOP (1,4-bis(5-phenyloxazol-2-yl)benzene)

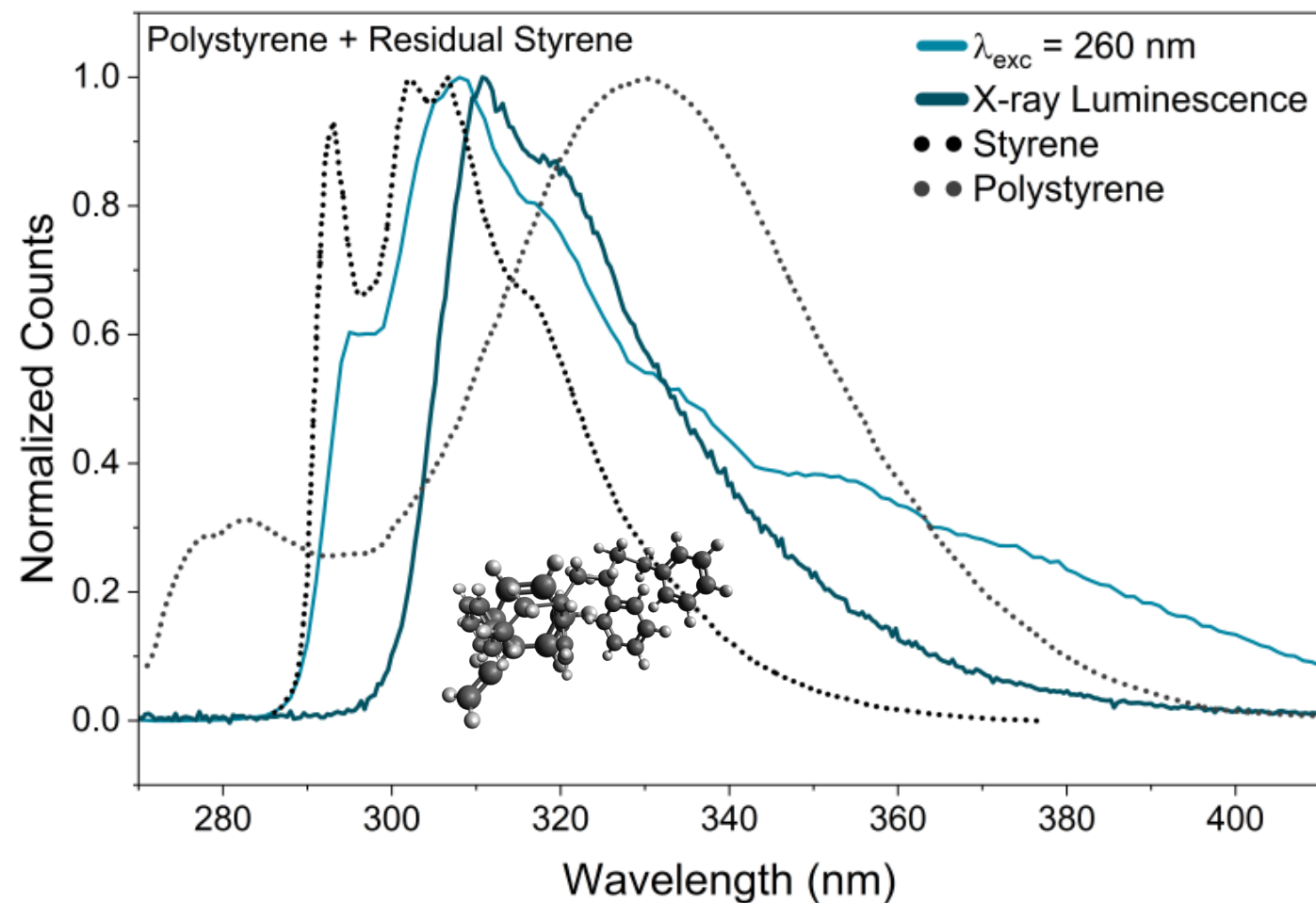
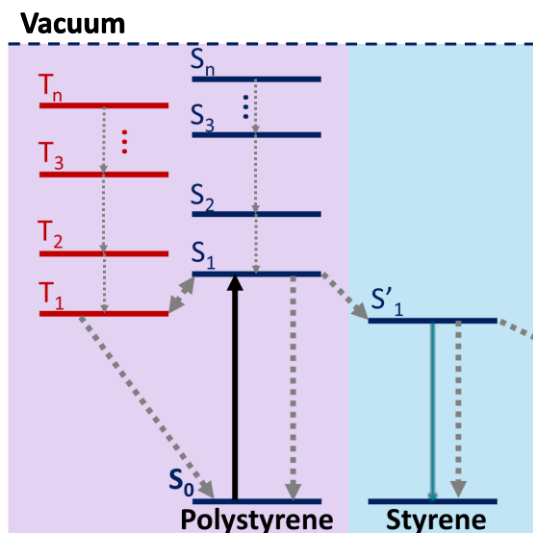


Bis-MSB (1,4-Bis(2-methylstyryl)benzene) 7

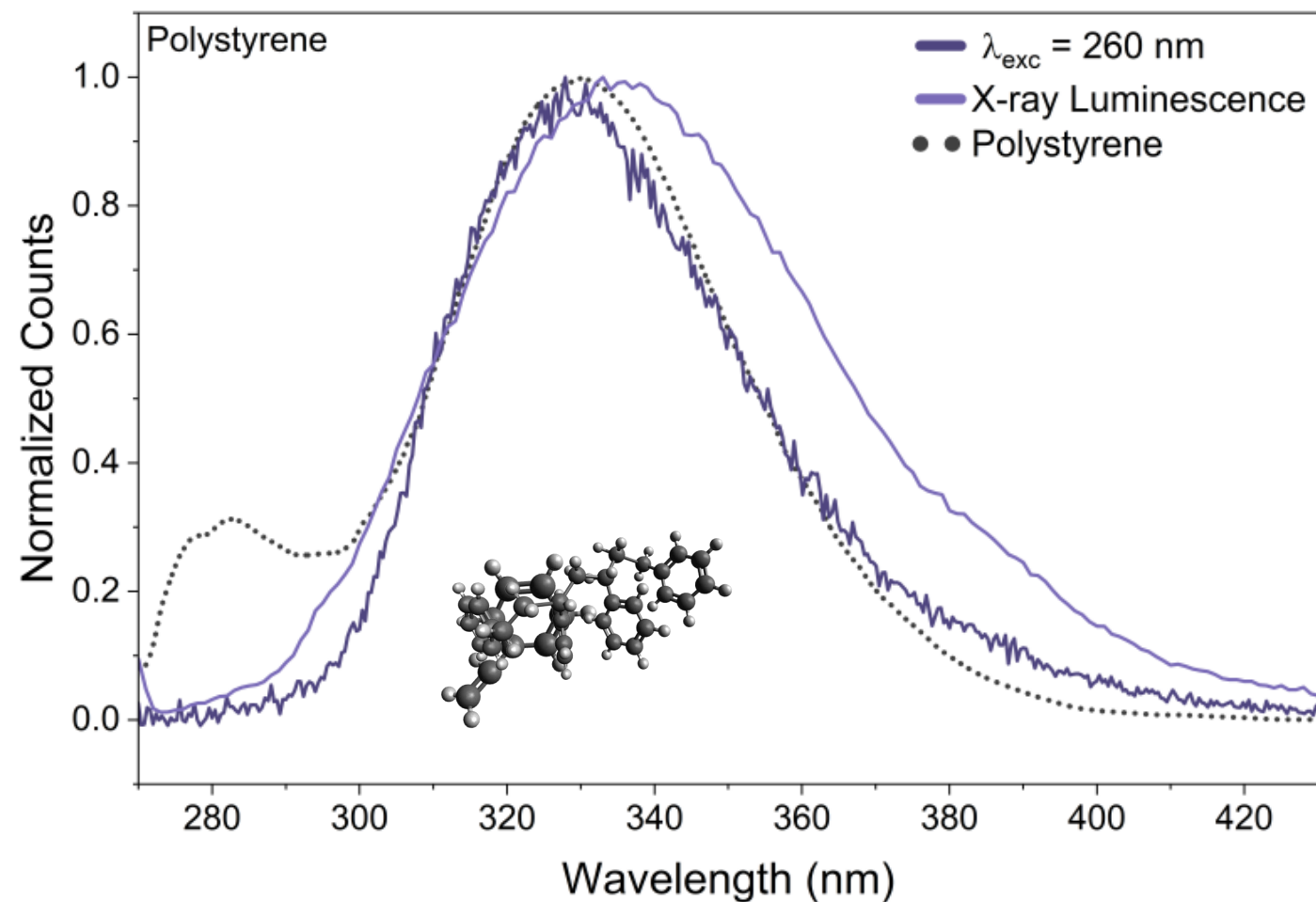
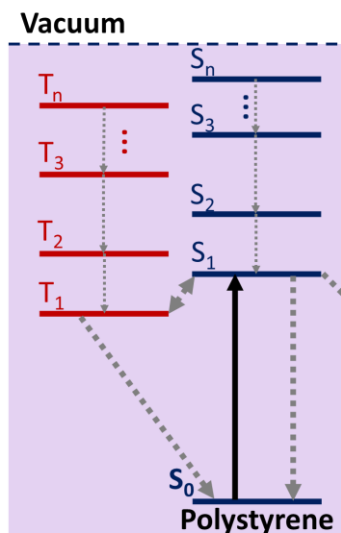
Sample	PS (g)	PPO (mg)	POPOP (mg)	Bis-MSB (mg)
1. PS	10	0	0	0
2. PS + 1% PPO	9.9	100	0	0
3. PS + 0.2% POPOP	9.98	0	20	0
4. PS + 0.2% Bis-MSB	9.88	0	0	20
5. PS + 1% PPO + 0.2% POPOP	9.98	100	20	0
6. PS + 1% PPO + 0.2% Bis-MSB	9.88	100	0	20

Steady State Spectra

1. Polystyrene
2. (Poly)styrene
3. (P)S + PPO
4. (P)S + POPOP
5. (P)S + Bis-MSB
6. (P)S + PPO + POPOP
7. (P)S + PPO + Bis-MSB

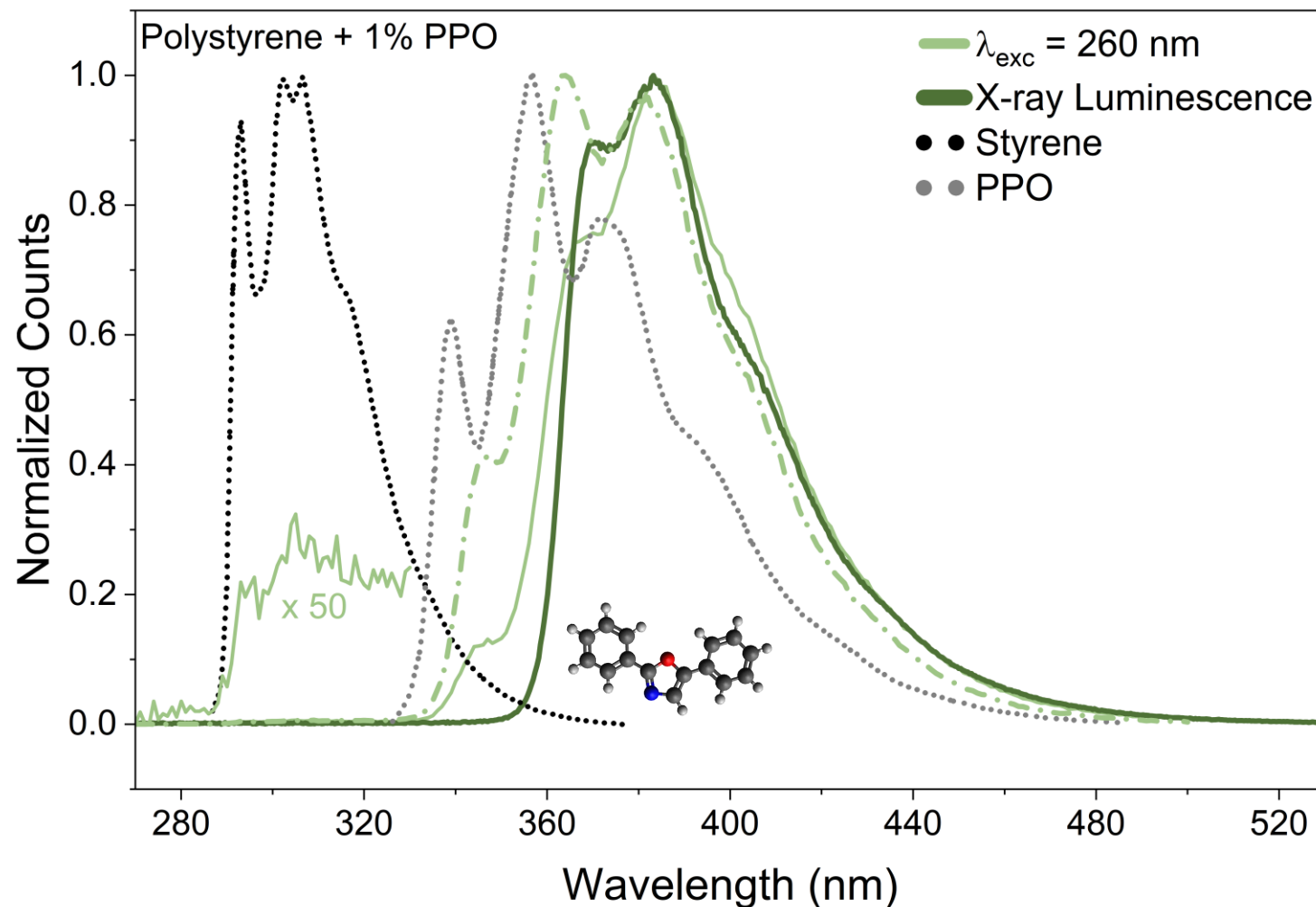
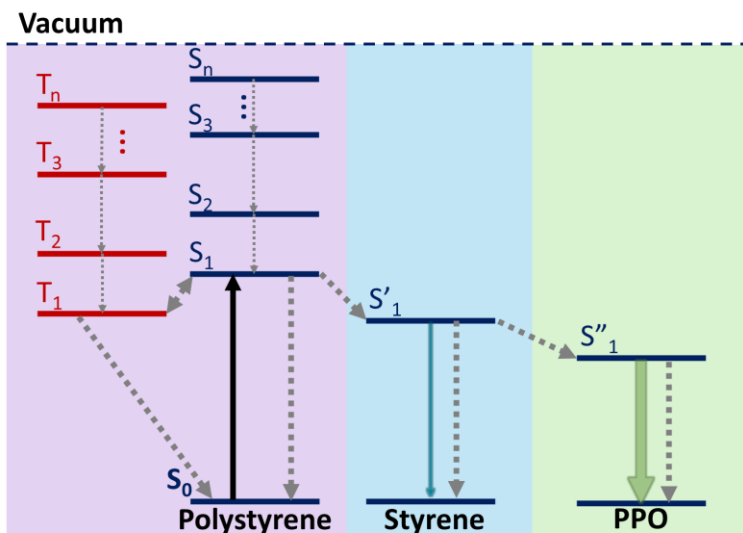


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5. (P)S + Bis-MSB
6. (P)S + PPO + POPOP
7. (P)S + PPO + Bis-MSB



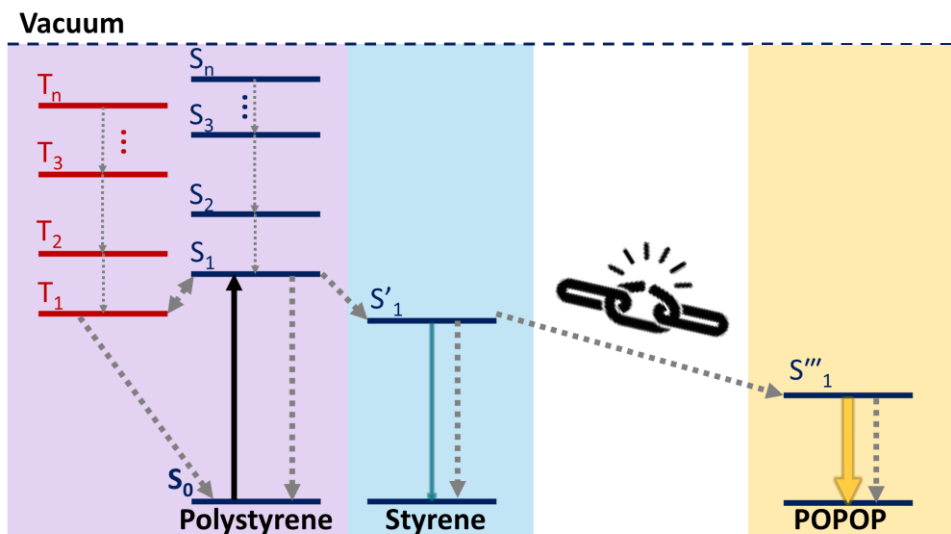
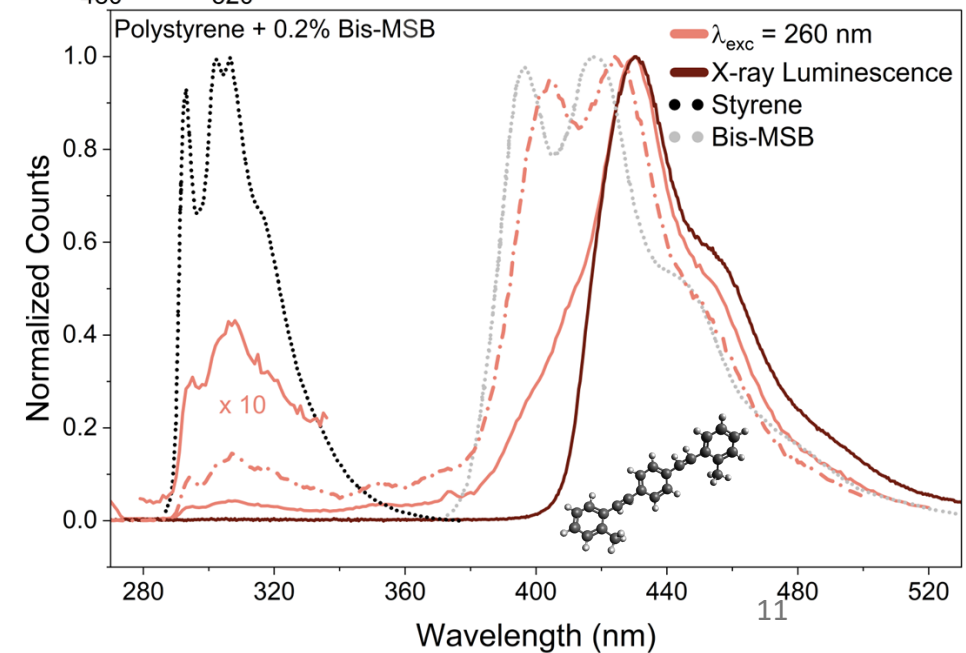
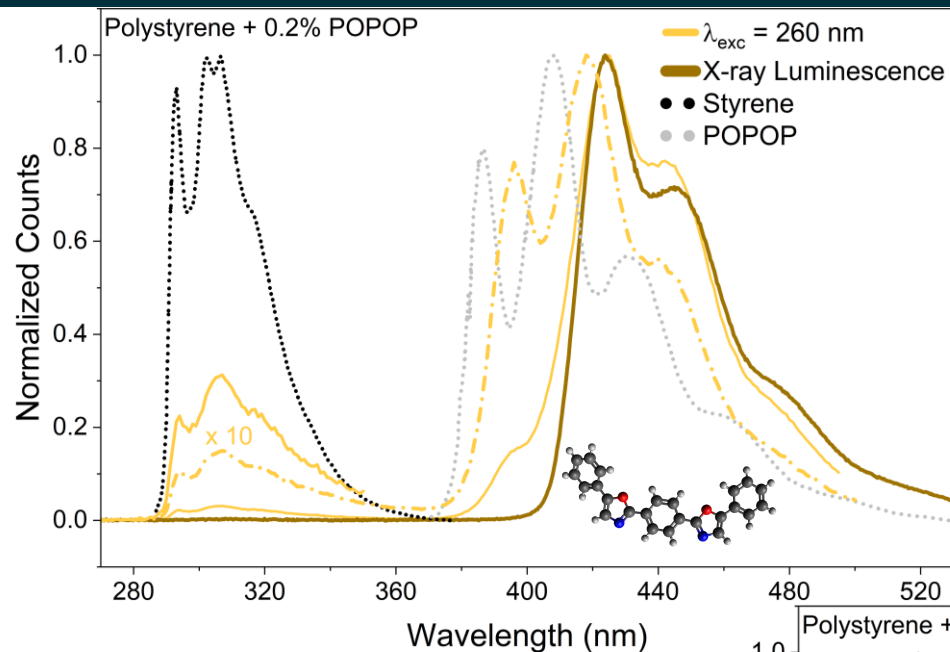
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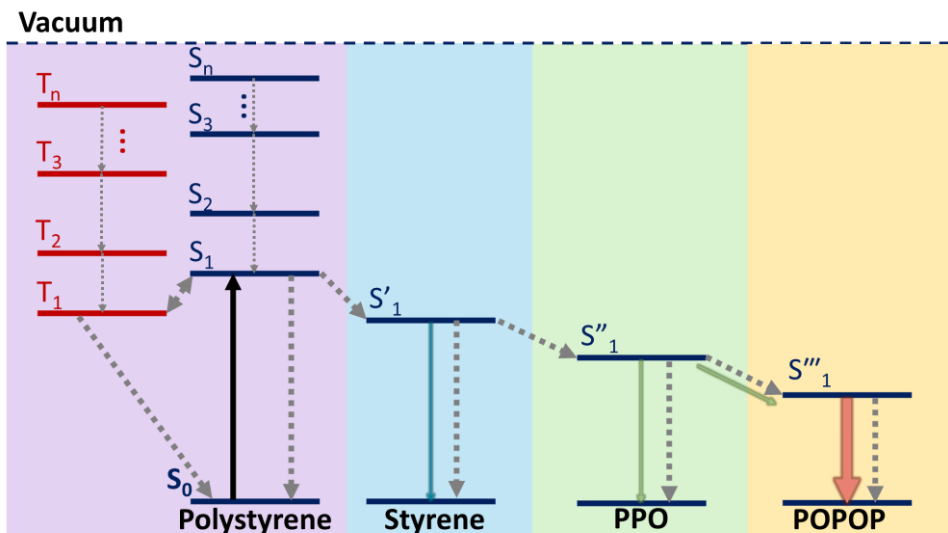
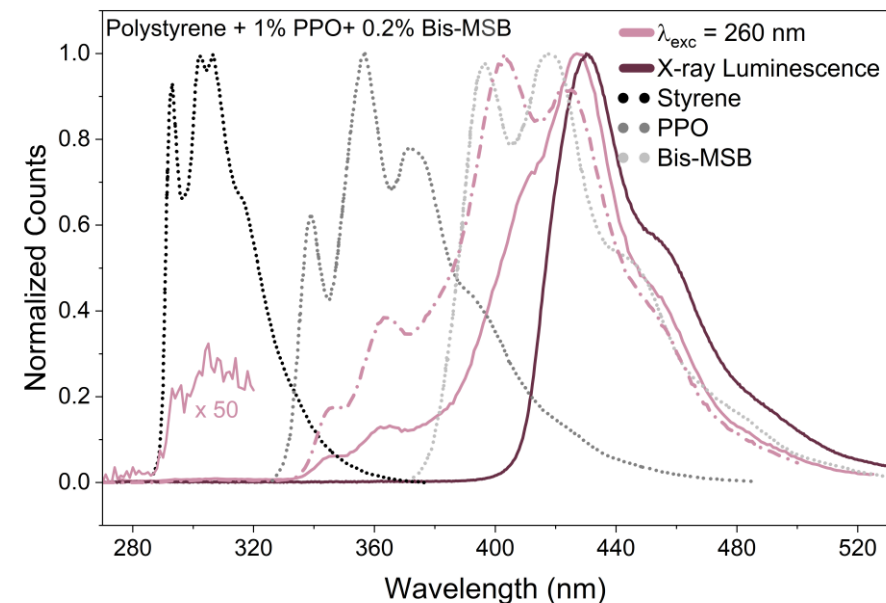
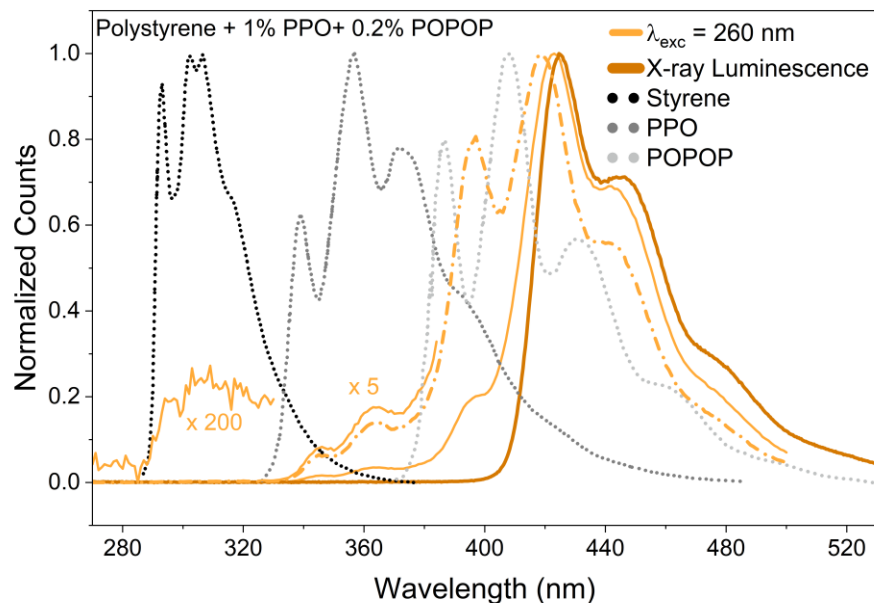
Steady State Spectra

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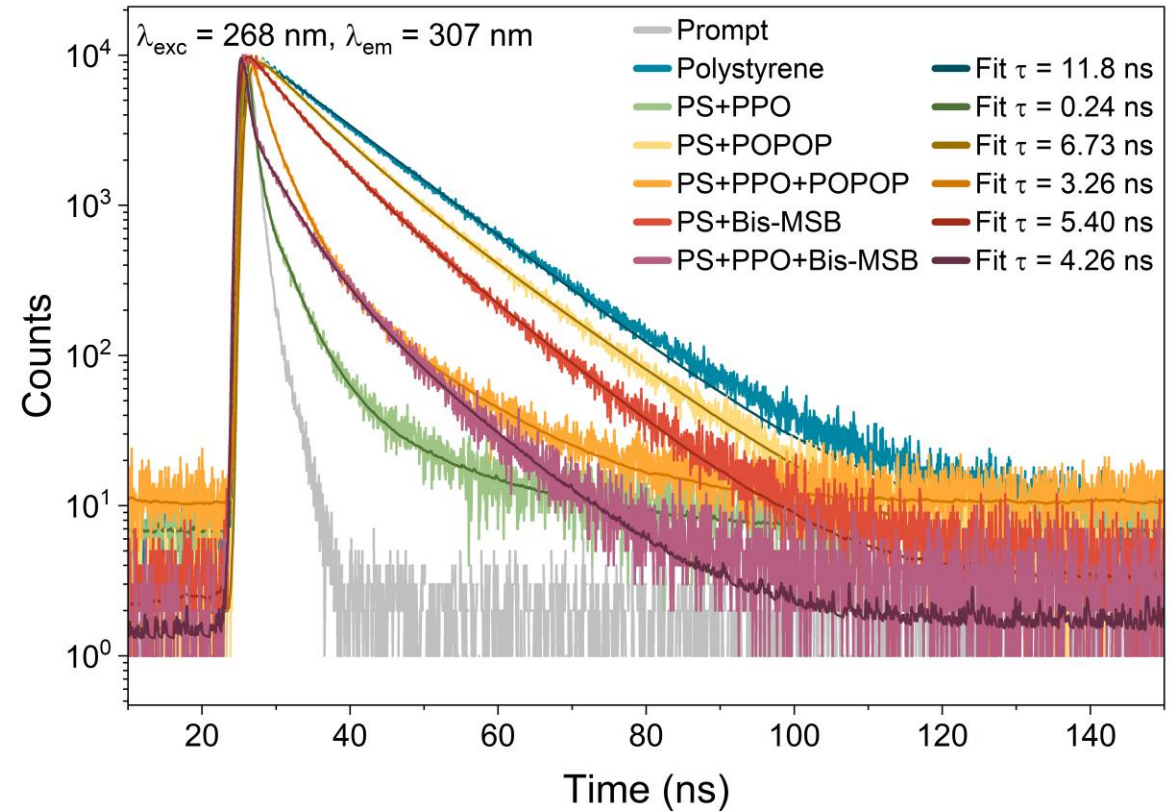
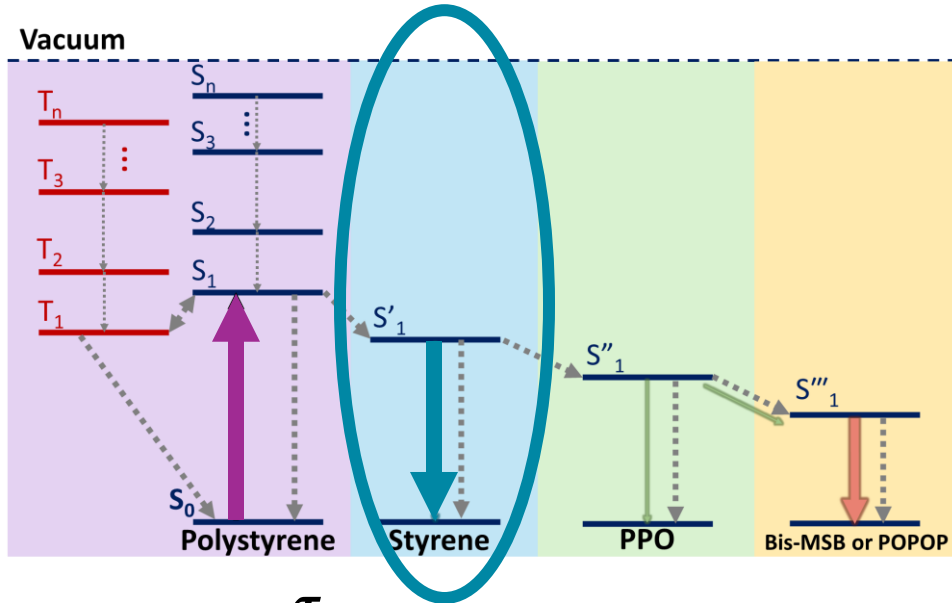
Steady State Spectra

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2. (Poly)styrene
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5. (P)S + Bis-MSB
6. (P)S + PPO + POPOP
7. (P)S + PPO + Bis-MSB



Scintillation spectra are more strongly affected by self-absorption, causing a UV cutoff.
 Scintillation emission spectrum is dominated by the lowest energy dye.

Decay of the Styrene Emission and Energy Transfer Efficiencies



$$\eta_{ET} = 1 - \frac{\tau_{DA}}{\tau_D}$$

$$\eta_{St \rightarrow PPO} = 98.0\%$$

$$\eta_{St \rightarrow POPOP} = 43.0\%$$

$$\eta_{St \rightarrow Bis-MSB} = 46.6\%$$

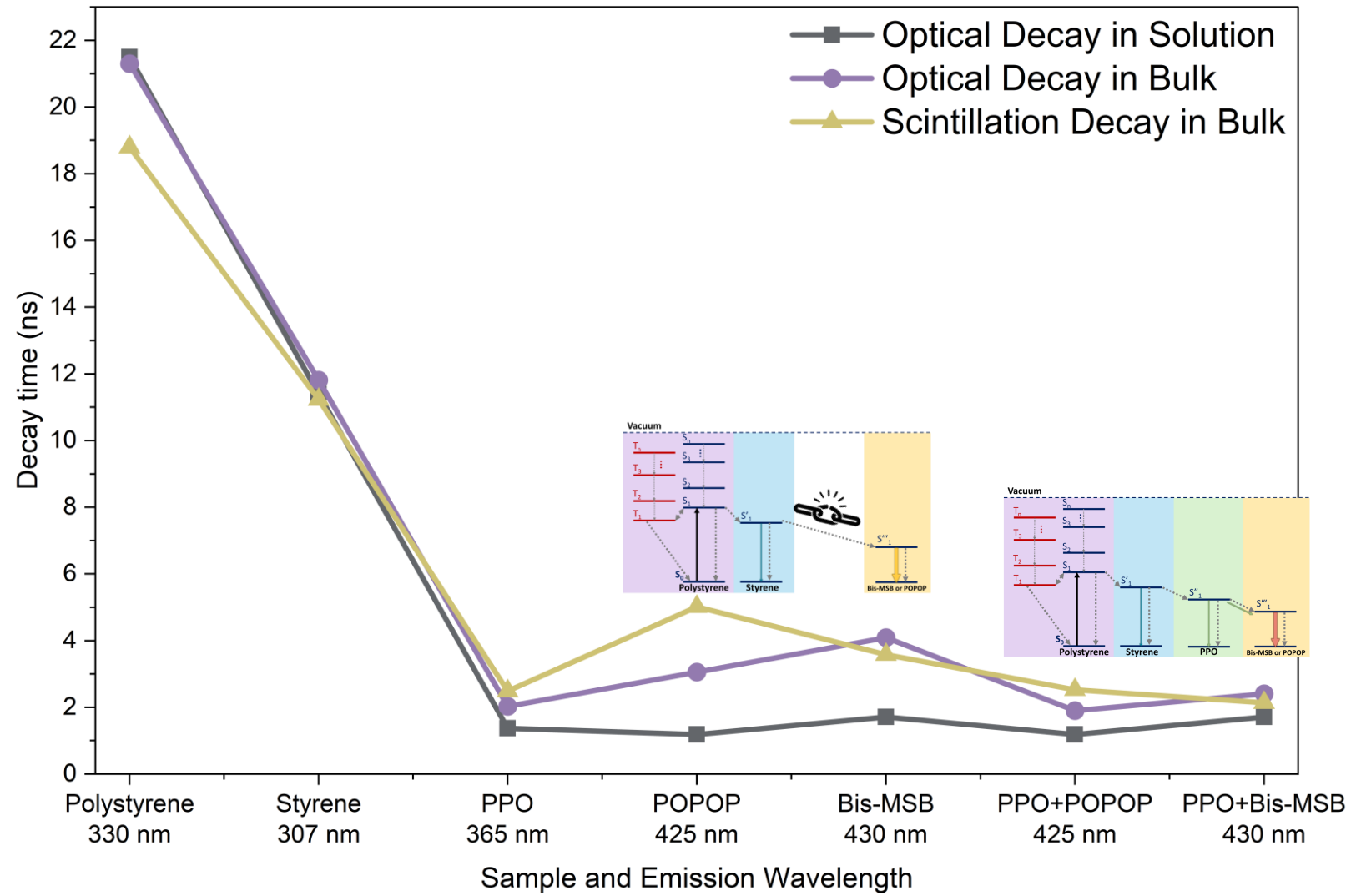
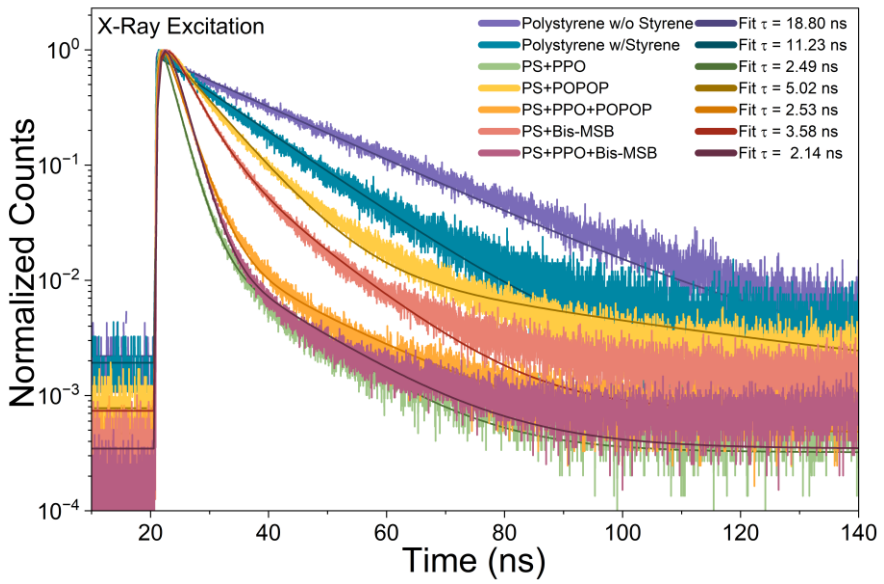
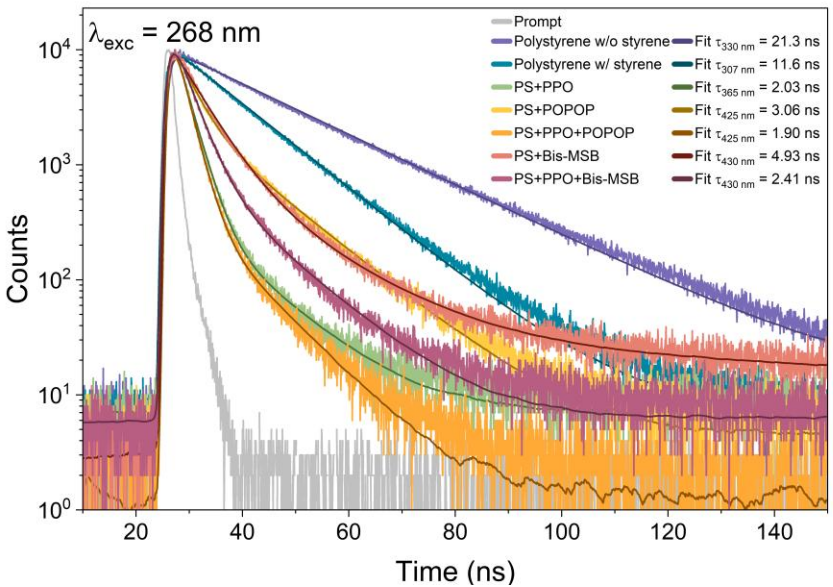
$$\eta_{St \rightarrow PPO+POPOP} = 72.4\%$$

$$\eta_{St \rightarrow PPO+Bis-MSB} = 63.3\%$$

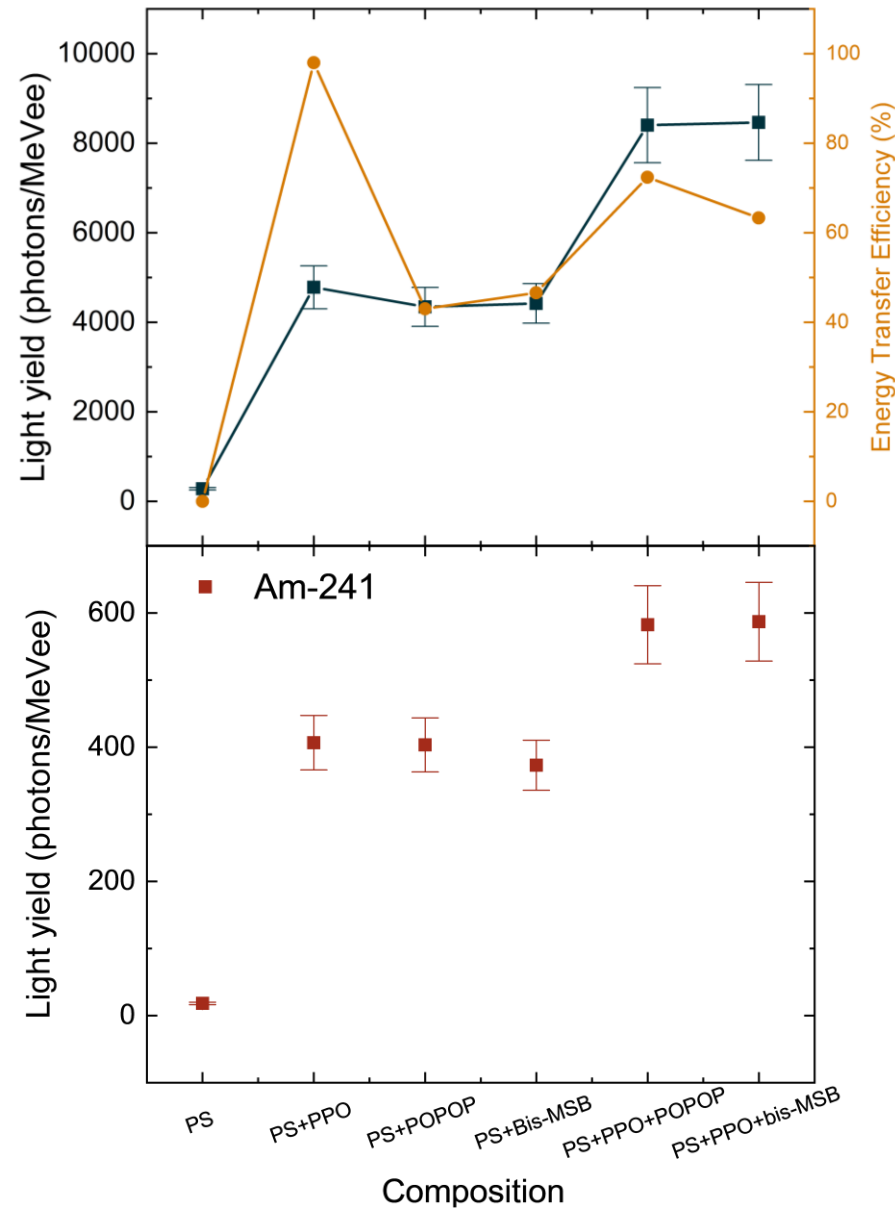
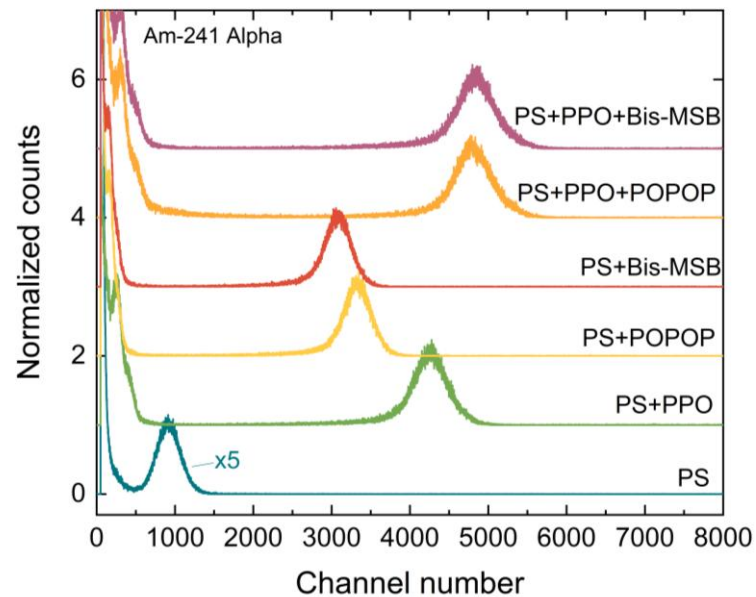
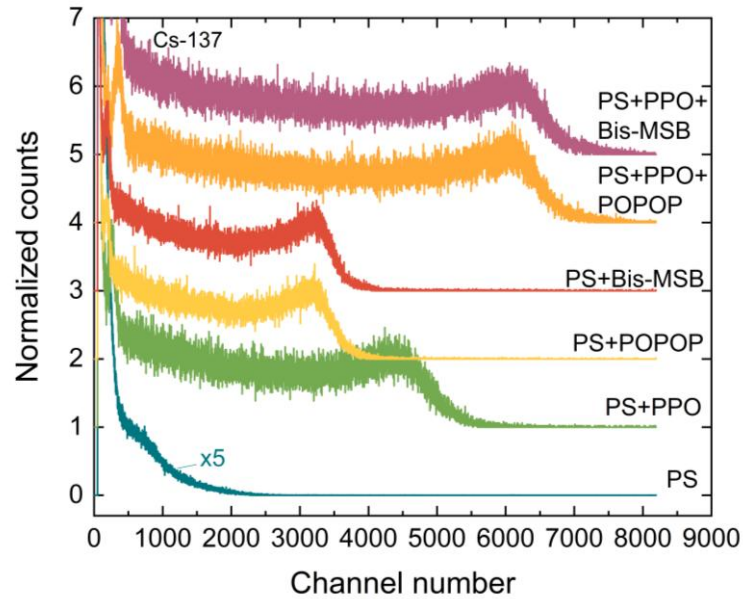
Styrene participates in the energy transfer chain due to efficient coupling to PPO.

PL can be used to probe earlier stages of energy transfer and determine its efficiency.

Optical Excitation Decay vs Scintillation Decay



Light Yield Measurements



Singly doped samples behave similarly

Co-doping nearly doubles the light yield.

POPOP and Bis-MSB have comparable light yields.

Light yield does not correlate with energy transfer efficiency.

- What are the advantages of using optical techniques?
 - PL can be used to shine light on earlier processes using tunability of excitation energies.
 - PL decay can be used to estimate energy transfer efficiency between host and solvents.
- What we learned?
 - PL decay can be used to estimate scintillation decay.
 - Breaking the energy transfer chain reduces energy transfer efficiency and light yield and slows scintillation decay time.
 - Co-doping increases light yield but reduces the energy transfer efficiency from styrene.
- What is next?
 - Understanding the role of residual styrene by removing it or measuring the amount.
 - Varying dopant concentration to better understand their roles.

A photograph of four people standing outdoors in front of a large tree and a wooden bench. From left to right: a woman in a light blue sweater with pink polka dots and blue jeans; a woman in a bright pink coat over a white sweater and patterned leggings; a man in a dark blue hoodie and dark pants; and a woman in a white and brown sweater vest over a dark top and dark pants. The word "Questions?" is overlaid in large white text across the center of the image.

Questions?