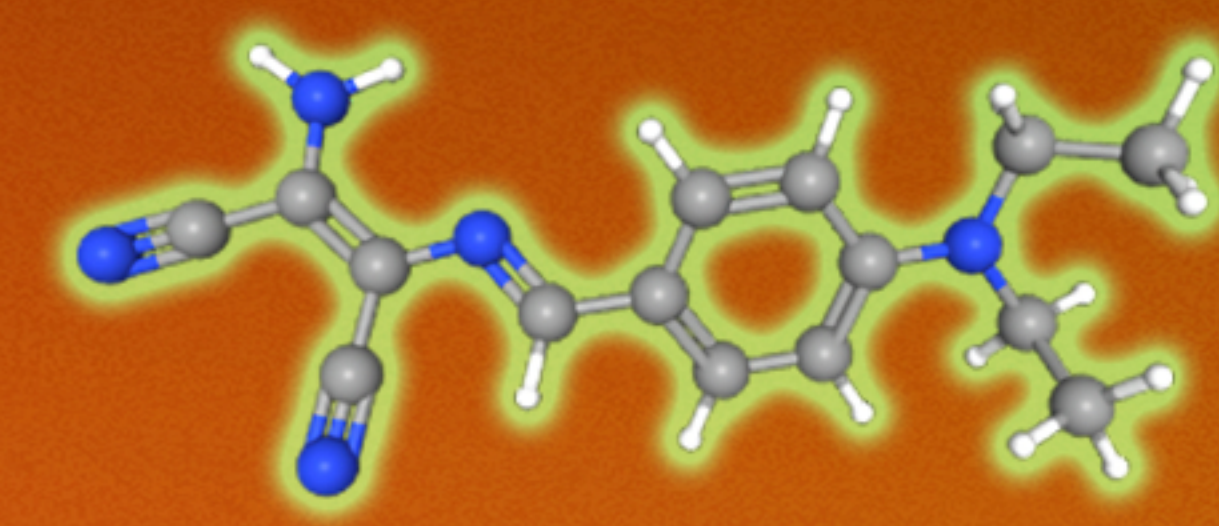


Investigating Dissolution Dynamics of Aggregation-Induced Emission Molecules for Efficient Optoelectronic Applications

Susith Mendis & Neranga Abeyasinghe*

Department of Chemistry, Faculty of Science, University of Colombo, Sri Lanka

*neranga@chem.cmb.ac.lk



UNIVERSITY OF
C O L O M B O



Commonwealth
Chemistry
Federation of Chemical Sciences Societies

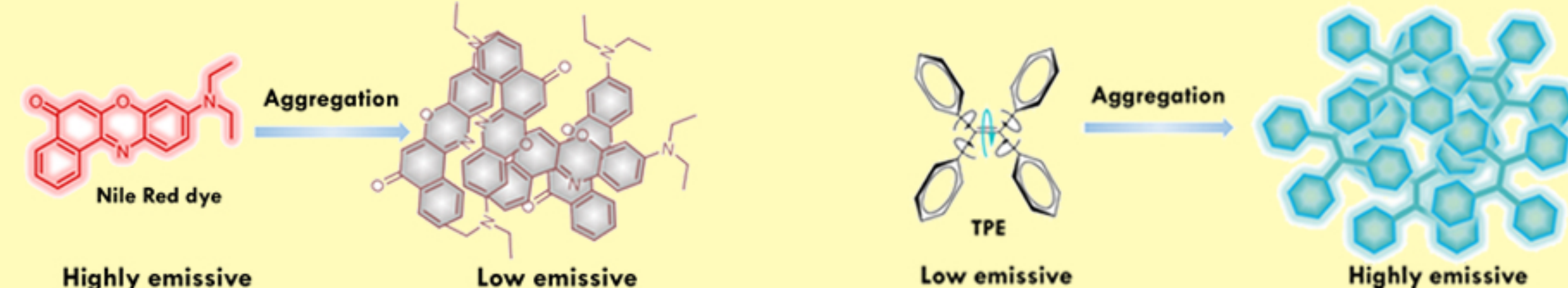


INTRODUCTION

Aggregation-induced emission (AIE): Traditional fluorescent materials dim when clustered (aggregation-caused quenching (ACQ)), but AIE molecules like A3MN glow brighter in groups — ideal for real-world devices.

Focus molecule: A3MN (2-Amino-3-((E)-(4-(diethylamino)benzylidene)amino)maleonitrile), a donor- π -acceptor structure with ICT potential.

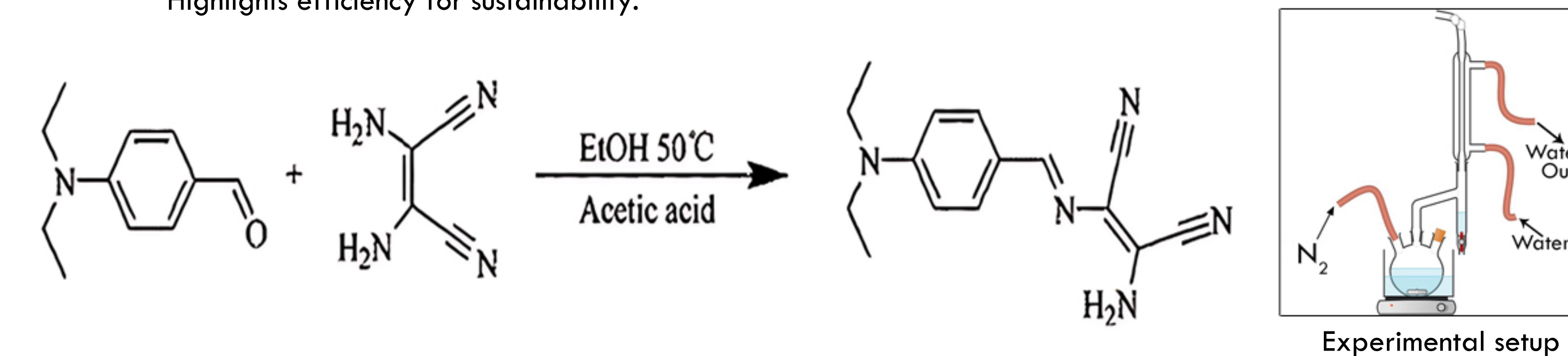
Research focus: Synthesis of A3MN, its optical properties, and dissolution dynamics (how it dissolves and affects light emission in different solvents/crystal forms).



METHODS AND TECHNIQUES

Materials: Diaminomaleonitrile, 4-diethylaminobenzaldehyde, absolute ethanol (dried with 3Å sieves), nitrogen atmosphere.

Synthesis: One-step Schiff base condensation reaction under mild conditions; purification via recrystallization in THF/ethanol. Highlights efficiency for sustainability.

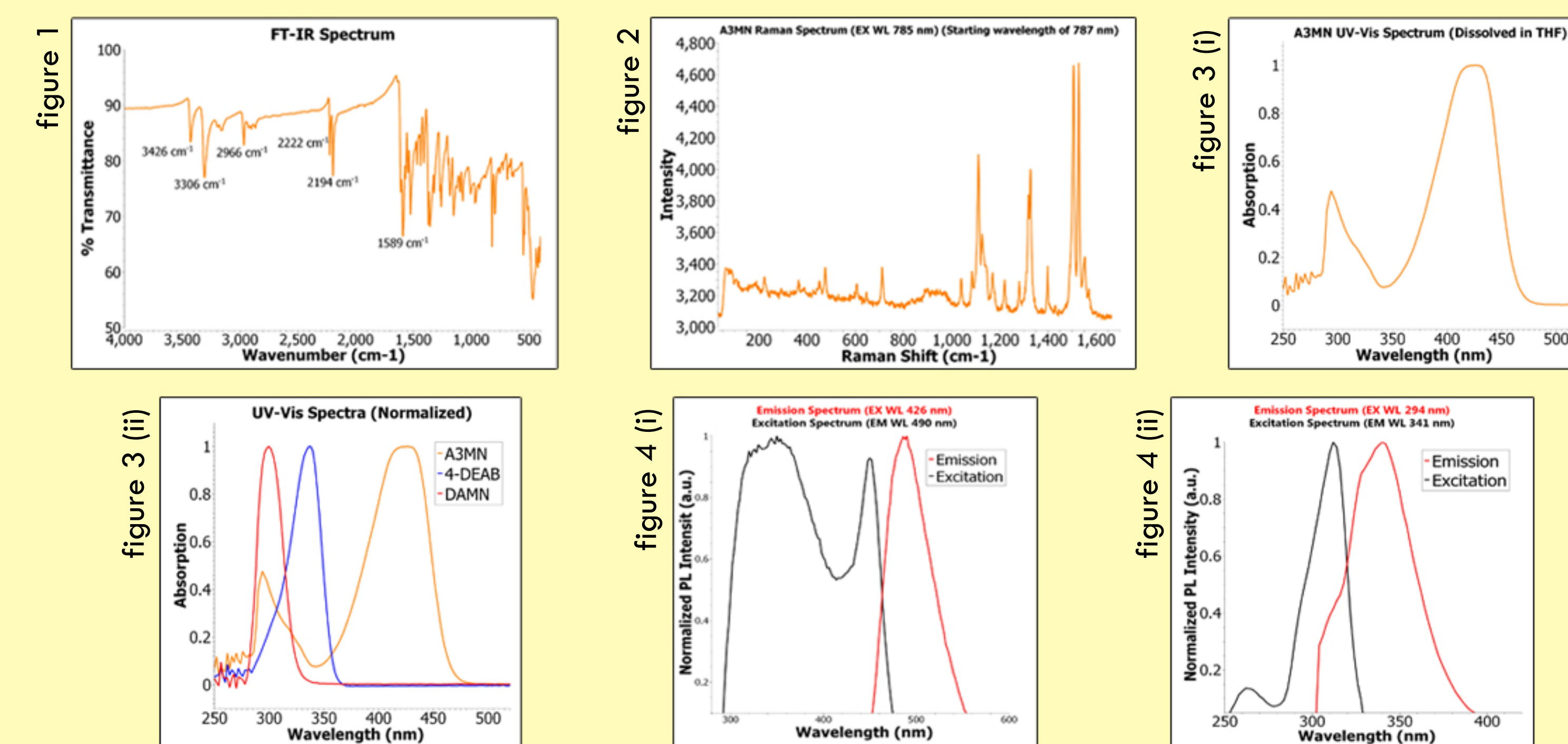


Optical investigations: FT-IR Spectroscopy for functional groups (imine, nitrile)
UV-Vis Spectroscopy for absorption (π - π^* , n- π^* transitions)
Raman Spectroscopy for vibrational modes (785 nm excitation)
Fluorescence Spectroscopy for emission/excitation spectra (time-resolved, 0-96h)

Dissolution studies: Visible solid particles (VSPs) were noted qualitatively as an initial indicator of aggregation
Time-dependent solubility in DMSO, ethanol, toluene, hexane, THF via spectroscopic methods
Physiochemical solvent properties (polarity, viscosity, dielectric constant, solvent-solute interactions)
Compared single vs. crushed crystals (ACS paper: TEM for nanoparticles)

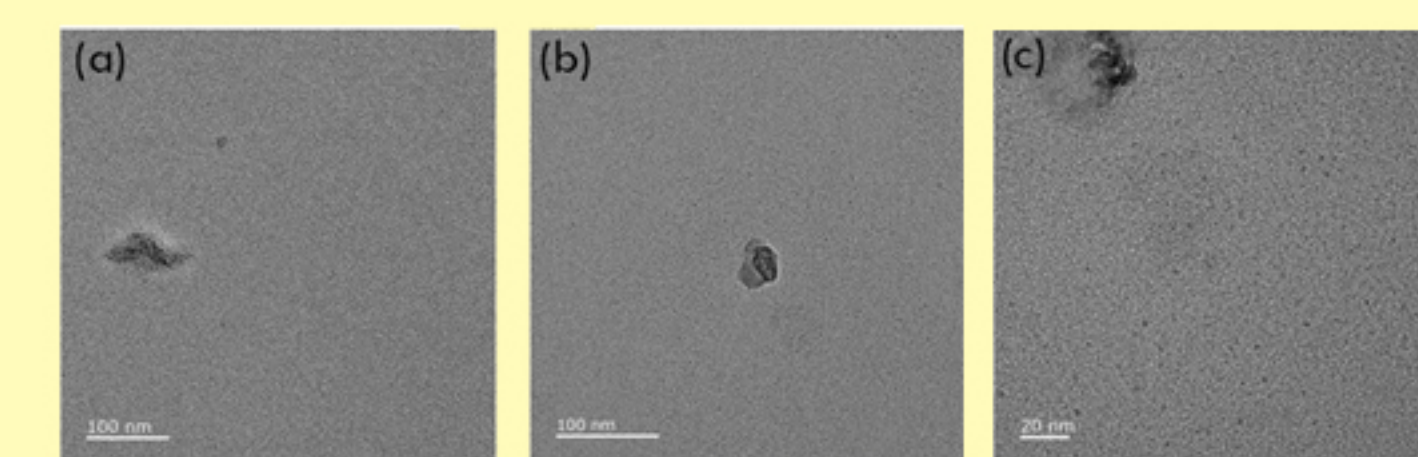
RESULTS AND DISCUSSION

Optical Properties: Confirmed structure with FT-IR (figure 1)/Raman (figure 2); UV-Vis (figure 3) showed ICT at 426 nm in THF; Fluorescence (figure 4) spectra shows dual emission behavior.

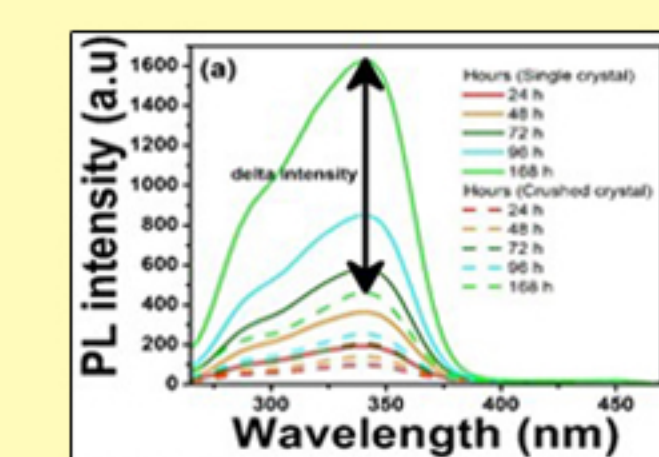


Dissolution Dynamics:

Single crystals dissolve faster than crushed in THF; crushed form nanosized particles (2-5 nm), slowing dissolution and fluorescence increase — shows "mechanical memory" effect.¹



TEM image of 37 nM solution of followings dissolved in THF after vacuum evaporation at 50 °C, (a) Single crystals. (b) Crushed single crystals (a large number of clearly dispersed A3MN particles are visible). (c) A zoomed-in TEM image for part of the field depicted in (b), where large numbers of clearly dispersed ~2–5 nm sized A3MN particles are visible.



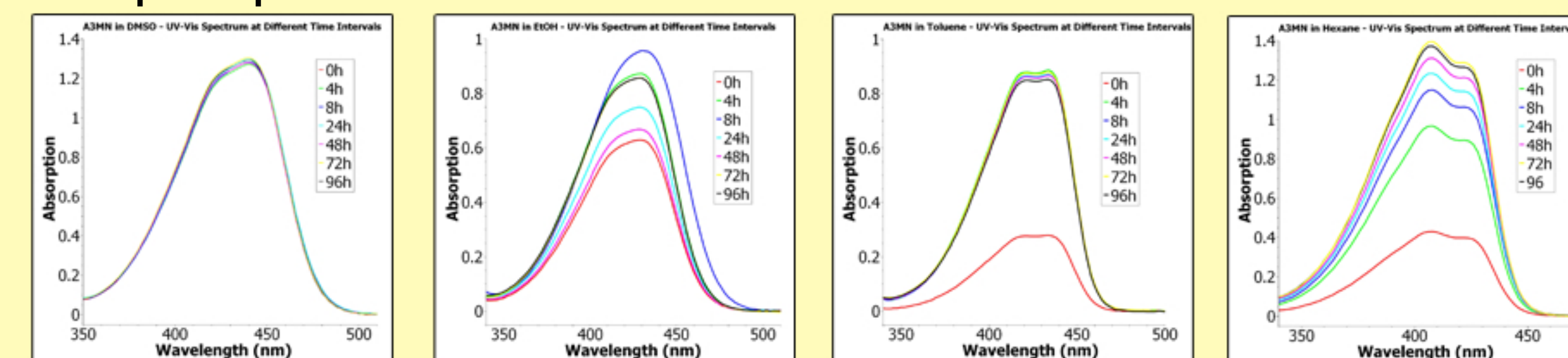
Excitation spectra for A3MN single crystals dissolved in THF (solid lines) and crushed single crystals (dashed lines) at different time intervals.

Time Dependent Solubility Dynamics:

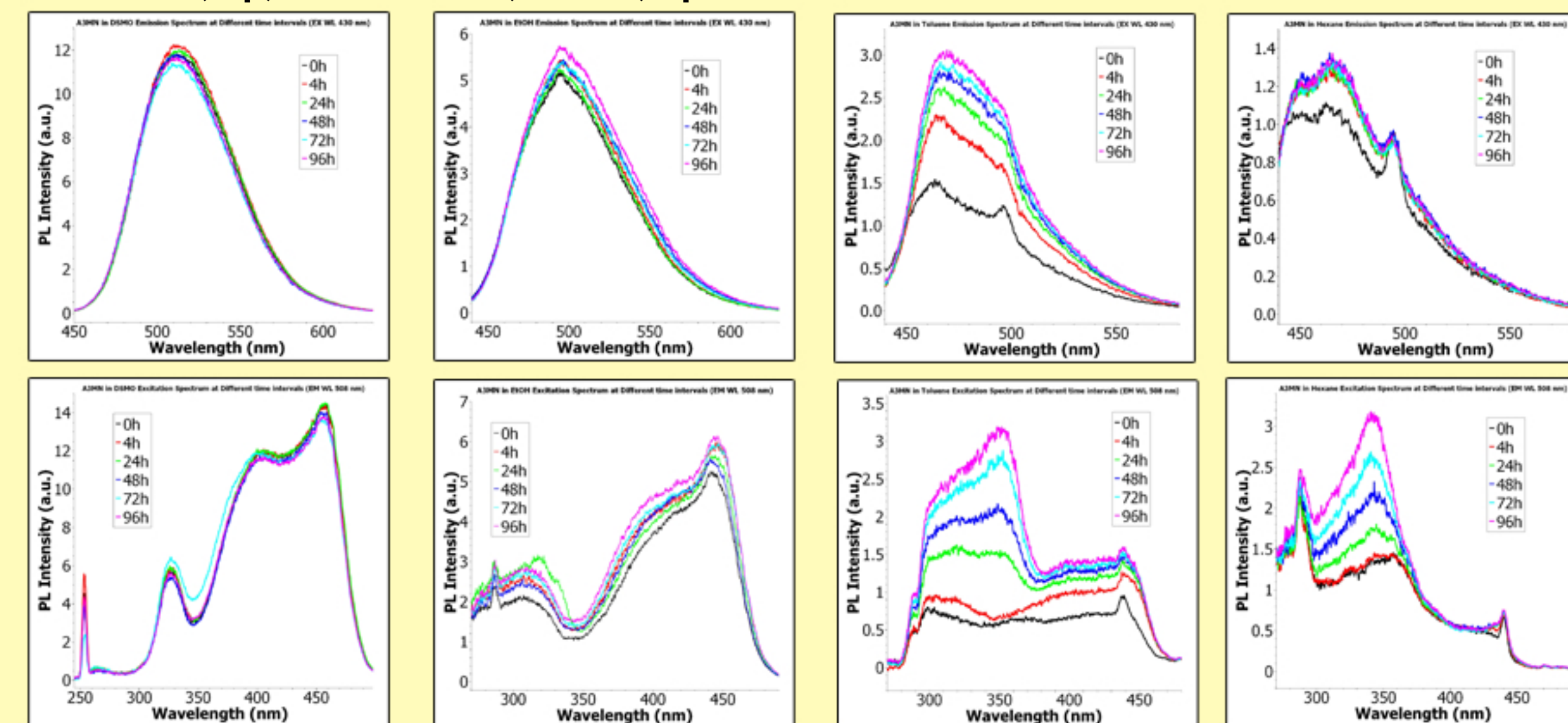
UV-Vis Absorption: Stable in DMSO over-time, Slowly stabilizes over-time in toluene and hexane.

Solvent-Dependent Emission: Red-shift in polar solvents (512 nm in DMSO) vs. blue-shift in nonpolar (466 nm in toluene/hexane) — links to tunable applications.

Absorption Spectra Over-Time



Emission (top) & Excitation (bottom) Spectra Over-Time



DMSO

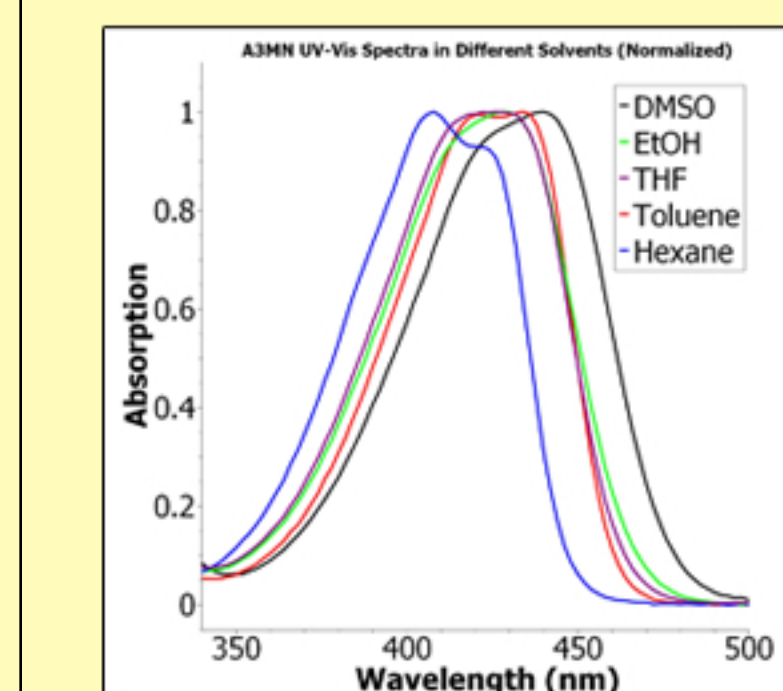
Ethanol

Toluene

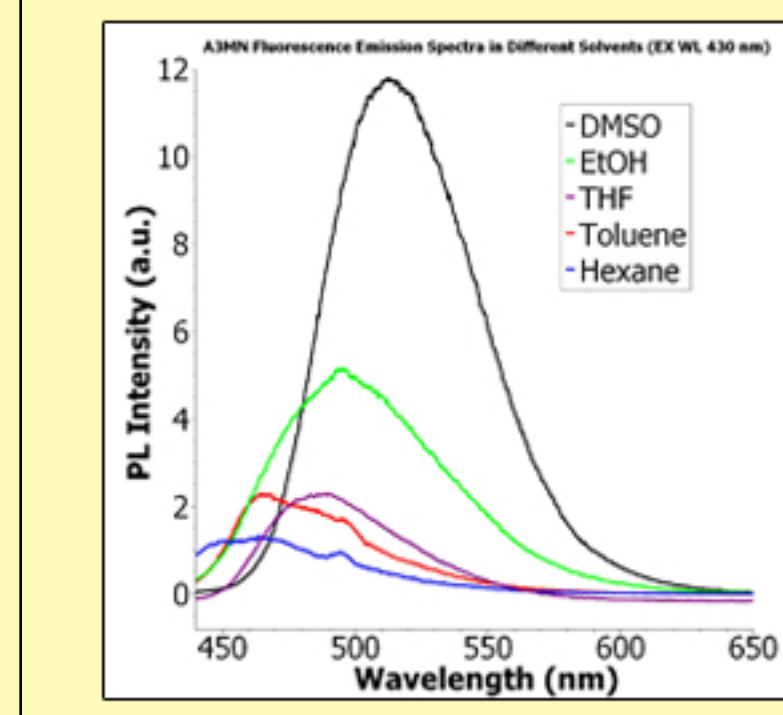
Hexane

Comparative analysis:

Spectra overlays show polarity effects (bathochromic in polar solvents); photostability in aggregates; implications for nonlinear optics (e.g., two-photon processes).



Normalized UV-Vis Absorption



Emission Spectra

APPLICATIONS AND IMPACT

Optoelectronics: AIE-enhanced emission for OLEDs (higher quantum yields, energy savings vs. traditional lighting); tunable for displays, sensors.

Sustainability: Mild synthesis reduces energy/waste; dissolution insights aid eco-friendly processing (e.g., non-toxic chemicals usage, nanoparticle control for stable devices).

SDG alignment: SDG 7 (affordable clean energy via efficient photonics); SDG 12 (responsible production through low-waste methods).

Broader potential: Bioimaging (high-contrast in aggregates), photodynamic therapy, molecular sensing.

CONCLUSION AND FUTURE WORK

Key findings: A3MN exhibits strong ICT, solvatochromic shifts, and morphology-dependent dissolution, enabling robust AIE for optoelectronics.

Impact: Contributes to AIE materials field; demonstrates potential for sustainable devices addressing energy challenges.

Limitations: Incomplete dissolution in nonpolar solvents; need for quantitative nonlinear data.

Future directions: Explore two-photon absorption, prototype OLED integration, computational modeling of ICT states; potential for diagnostics.

REFERENCES

- Senanayake, C. J.; Kavindi, T. D. D.; Deenalattha, D. H. S.; Arachchige, D. K.; Gunaratne, K.; Bandaranayake, P. M. A.; Rodrigo, U. D.; de Silva, N.; Abeyasinghe, N. Unveiling the Inversion-Symmetry-Driven Excitation Switching in Aggregation-Induced Emission. ACS Materials Letters 2025, 7 (5), 1930–1939.