Restriction of Twisted Intramolecular Charge Transfer (TICT) Enables the Aggregation-Induced Emission of 1-(N,N-Dialkylamino)-naphthalene Derivatives

Syed Ali Abbas Abedi*, Xiaogang Liu

Fluorescence Research Group

Singapore University of Technology and Design

syedaliabbas_abedi@mymail.sutd.edu.sg, xiaogang_liu@sutd.edu.sg

3rd Commonwealth Chemistry Posters
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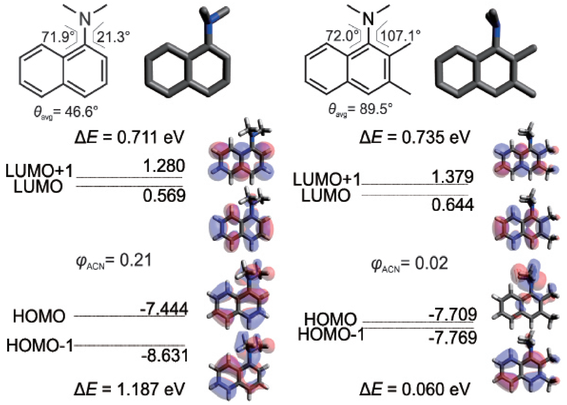
28-29 September 2022

ROYAL SOCIETY OF CHEMISTRY

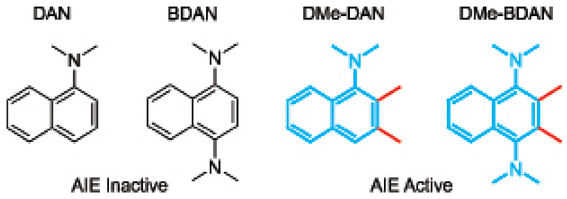
Introduction

By utilizing detailed quantum chemical calculations, we provide insights toward the Aggregation-Induced Emission (AIE) mechanism of DAN derivatives. Our theoretical analysis, corroborated by experimental observations, leads to the discovery that modulating the formation of the twisted intramolecular charge transfer (TICT) state (caused by the rotation of the amino groups) and managing the steric hindrance to minimize solid-state intermolecular interactions provides a plausible explanation for the AIE characteristics of DAN derivatives. These results will inspire the deployment of the TICT mechanism as a useful design strategy toward AIEgen development.

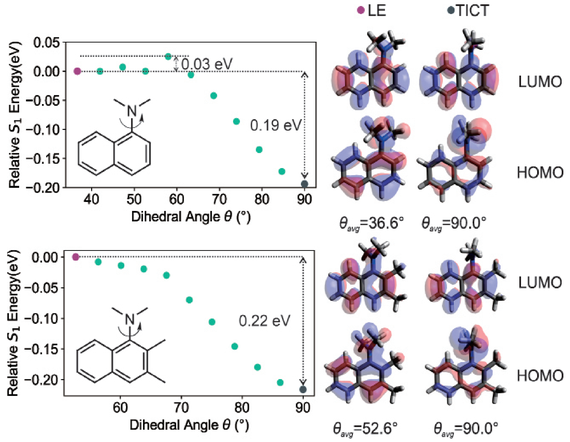
Influence of Steric Hindrance



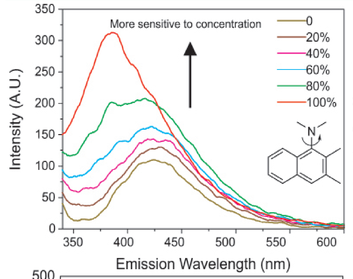
Compounds



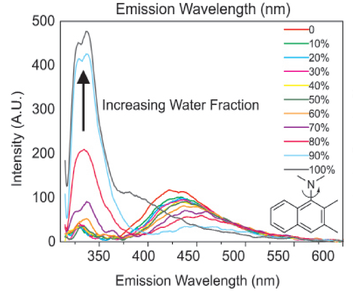
Methyl group induced strong TICT



Validation of TICT model



Viscosity test to restrict the rotations of diemethyl amino group in AIE active molecule (DMe-DAN) resulting in the recovery of fluorescence

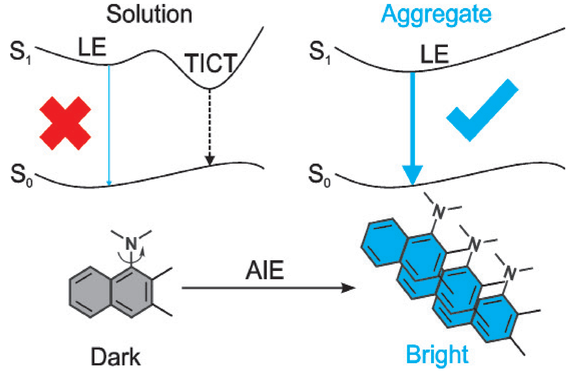


Aggregation test by adding water to the mixture and flouresscence intestity enhancement can be seen in DMe-DAN molecule

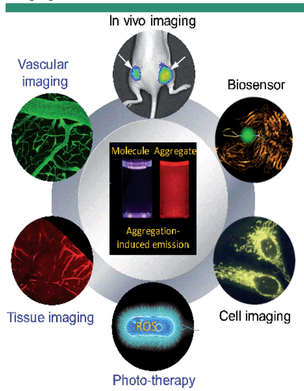
Conclusion

- Quantum computational chemistry aided to explore the structure-property relationship of fluorophores
- Rationalized AIEgens via TICT mechanism
- Mechanistic understanding could impove the AIEgens design for the future

Computational Strategy



Applications



- OLEDs
- DNA visualization
- Membrane imaging
- Bacteria imaging
- Ion detection
- Fingerprint visualization
- Sensors and probes

References

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