NREL
Transforming ENERGY

CO_2 Sorption in Aminopolymer-based Direct Air Capture Composites Through Fluorescent Detection

March 28th, 2023

Spring ACS Meeting

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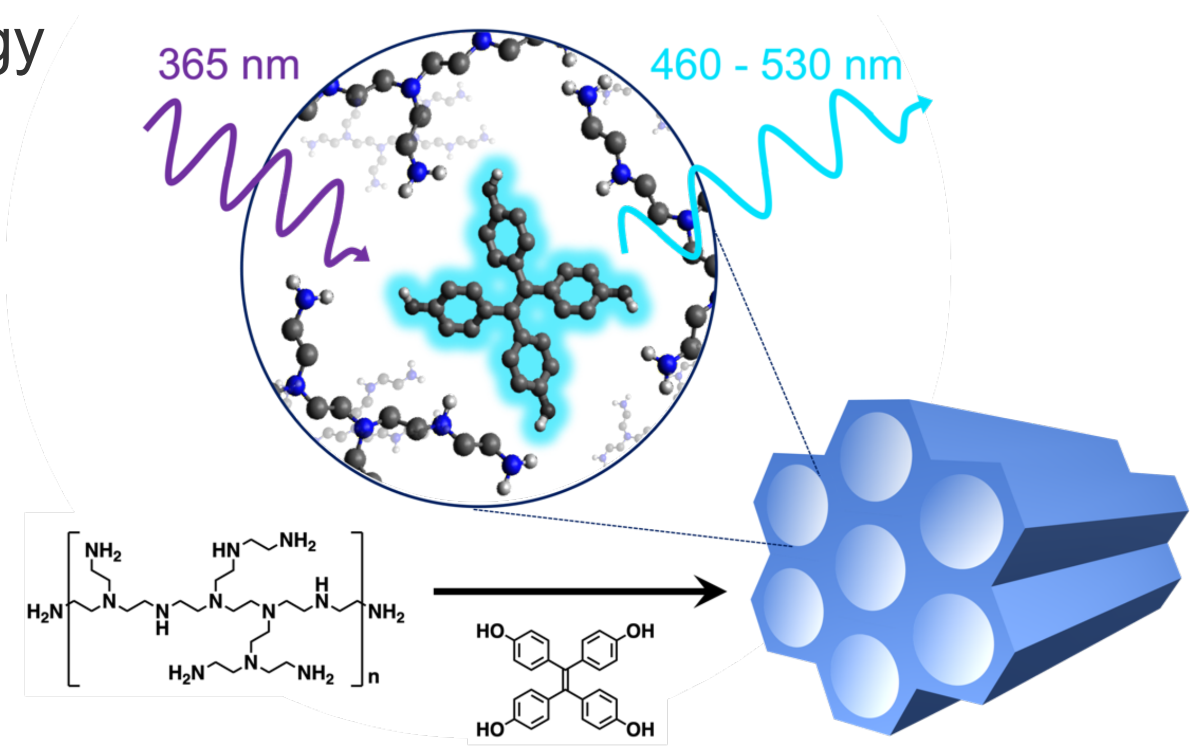
NREL/PR-5900-85774

Outline

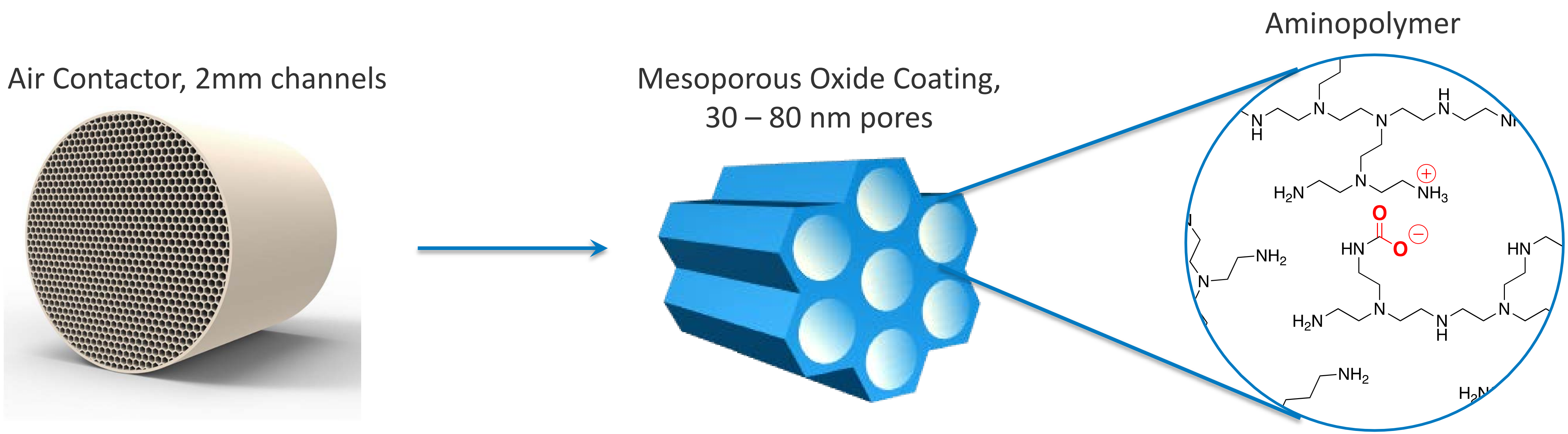
- Overview of Amine-Based DAC Technology
- Critical Role of Polymer Mobility
- Fluorescence for Probing Mobility
  - Mechanism
  - Benchmarking
  - CO_2 Uptake, Humid Environment
- Future Directions



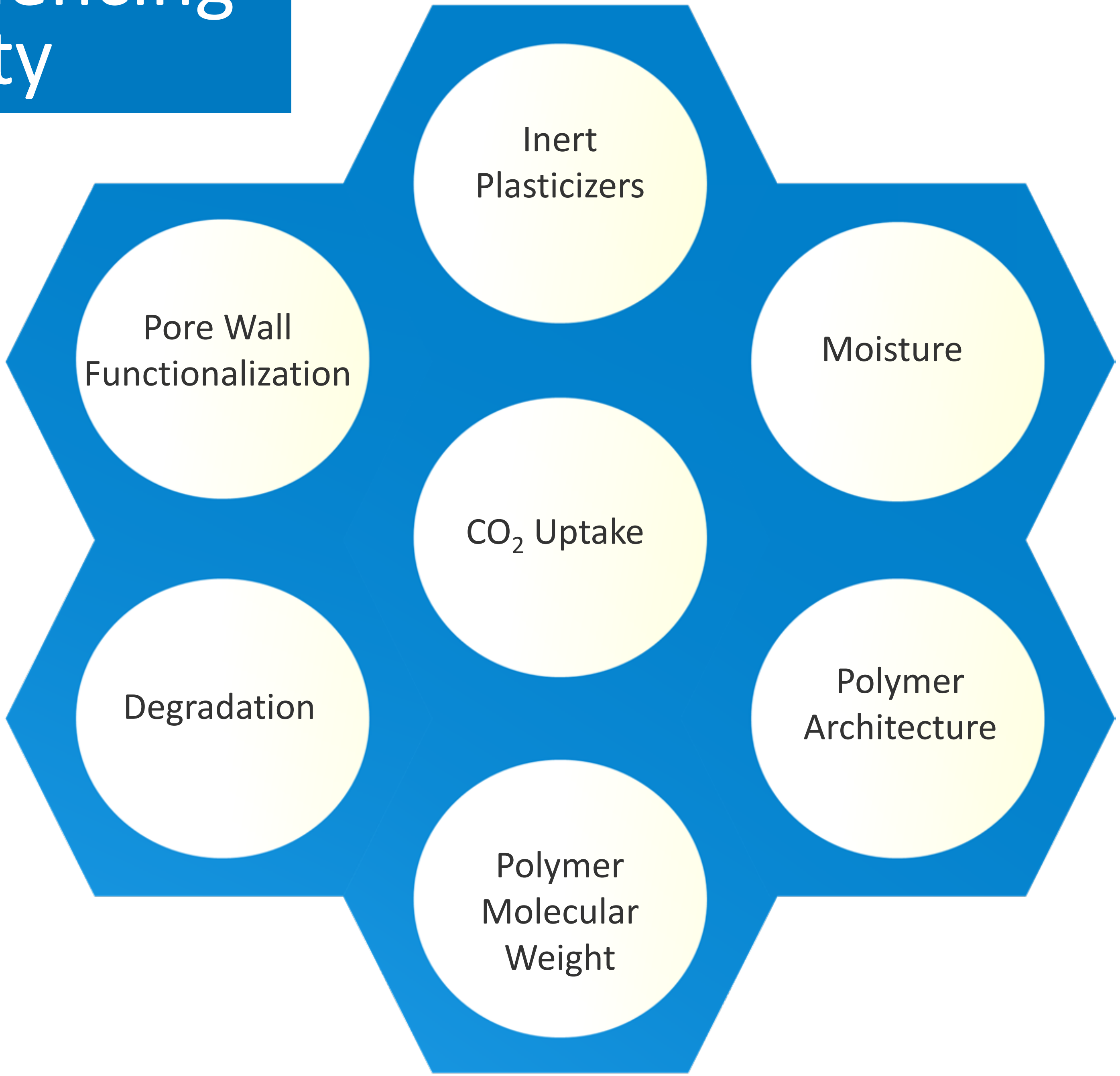
J. Phys. Chem. C., **2022**, 126, 10419.

https://doi.org/10.1021/acs.jpcc.2c01099

Amine-Based Direct Air CO_2 Capture



Factors Influencing Mobility



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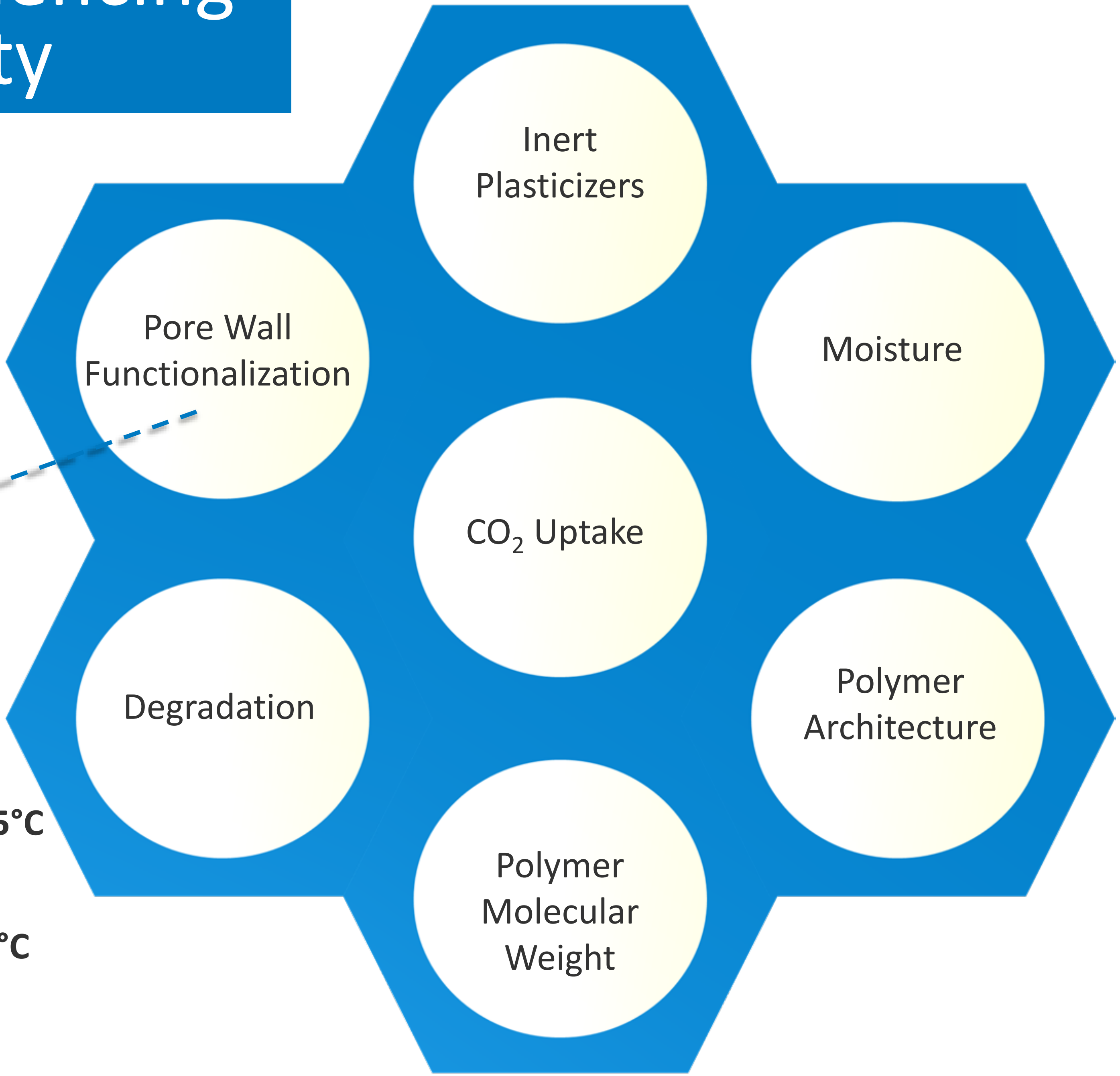
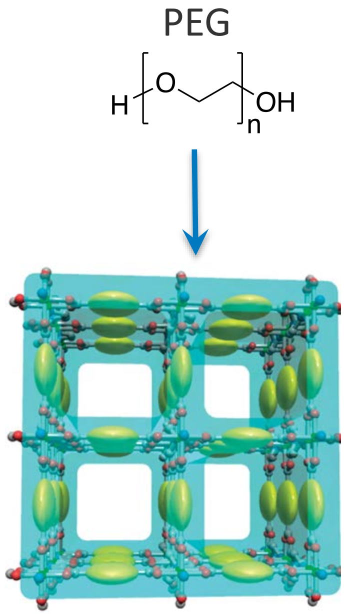
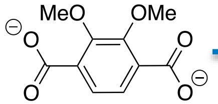
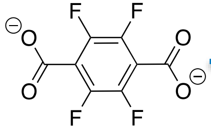






PEG T_g = +55°C



PEG T_g = -40°C

Nat. Commun. 2010, 1, 83.
https://doi.org/10.1038/ncomms1091

Factors Influencing Mobility

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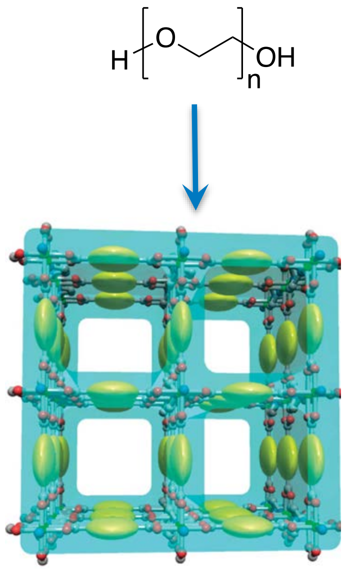

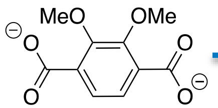

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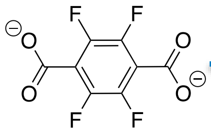

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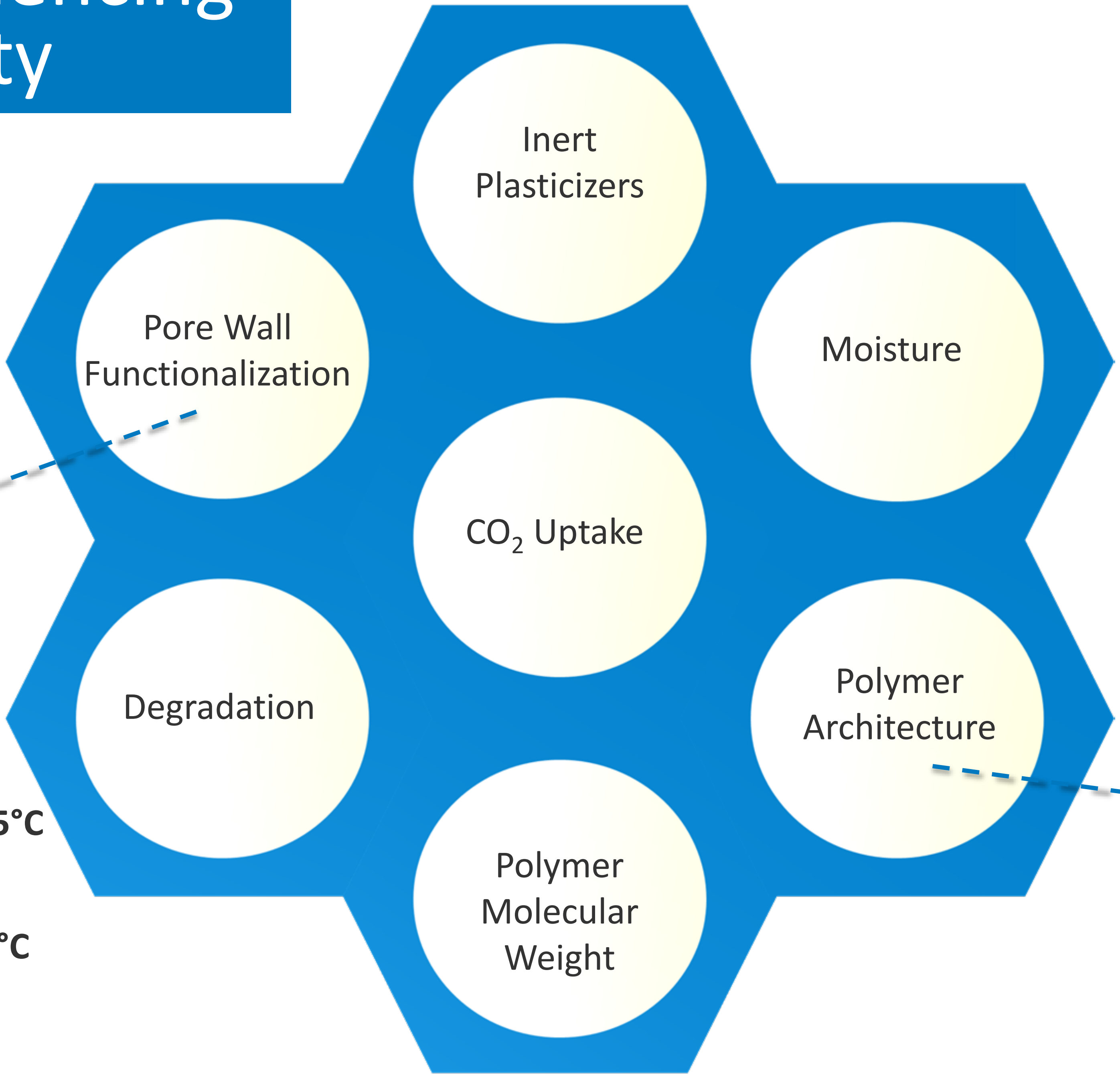
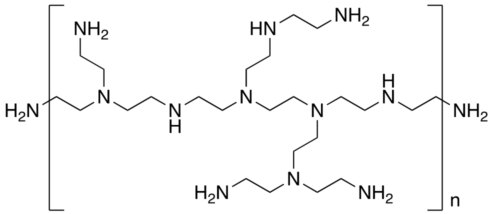
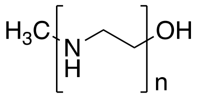




Branched PEI

T_g = -65°C



Linear PEI

T_m = +60°C

Factors Influencing Mobility

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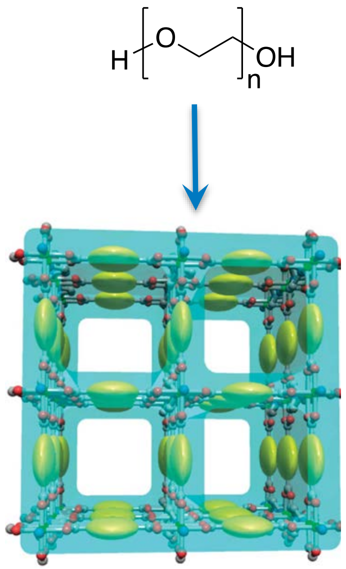

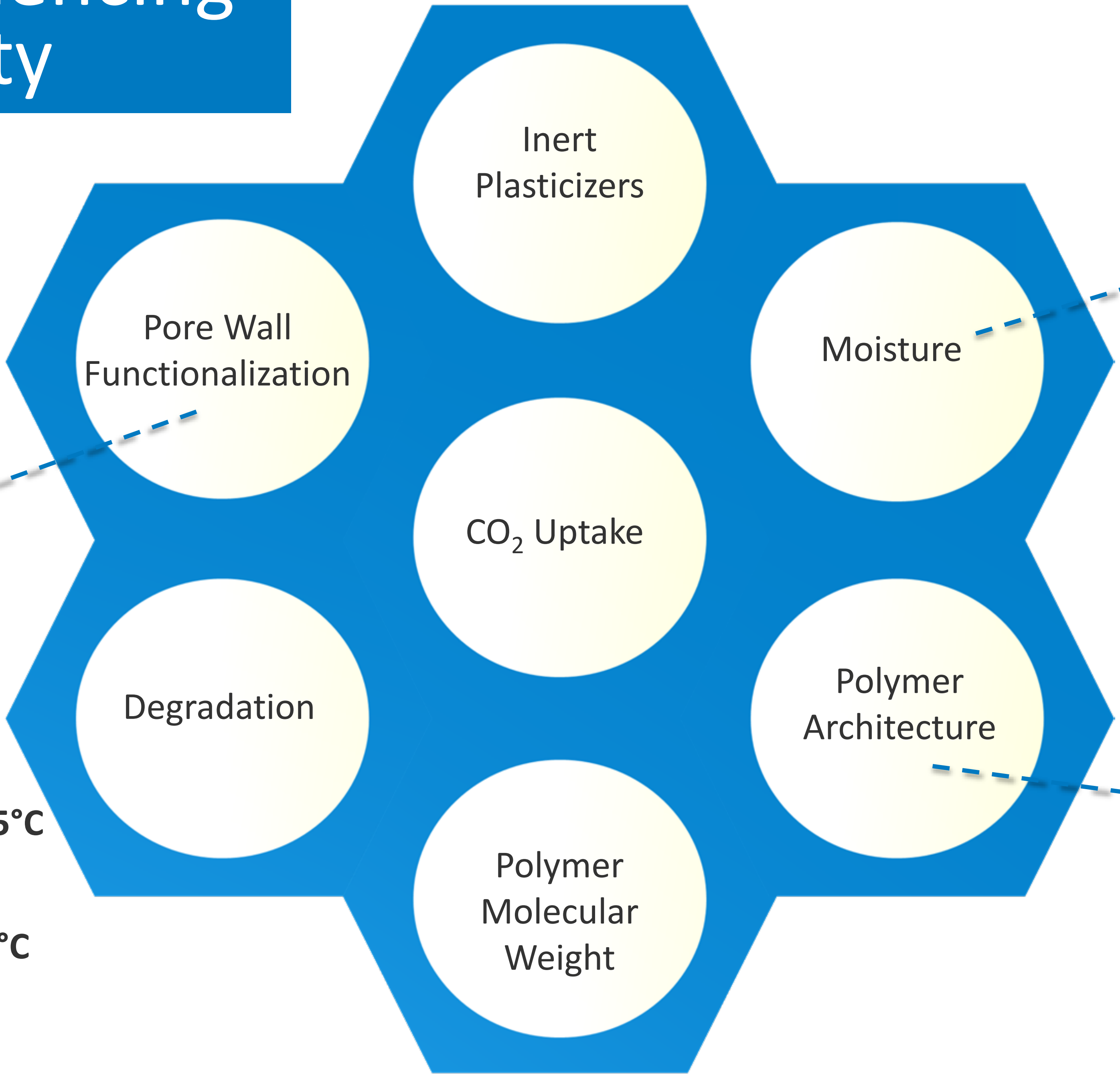

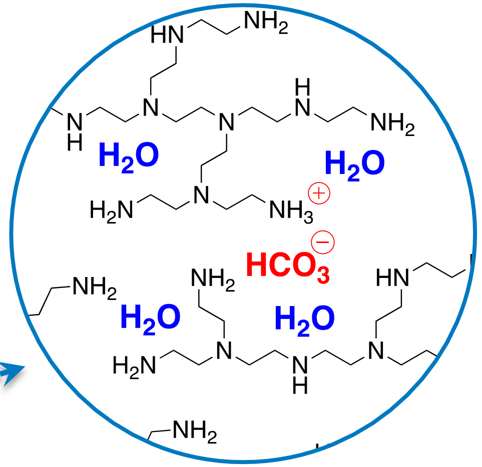

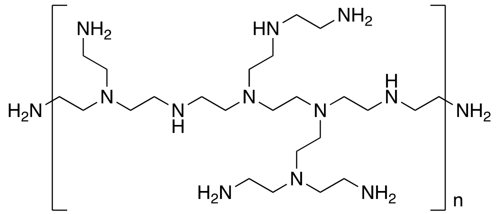

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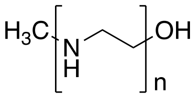

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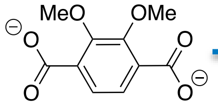

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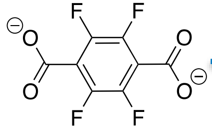

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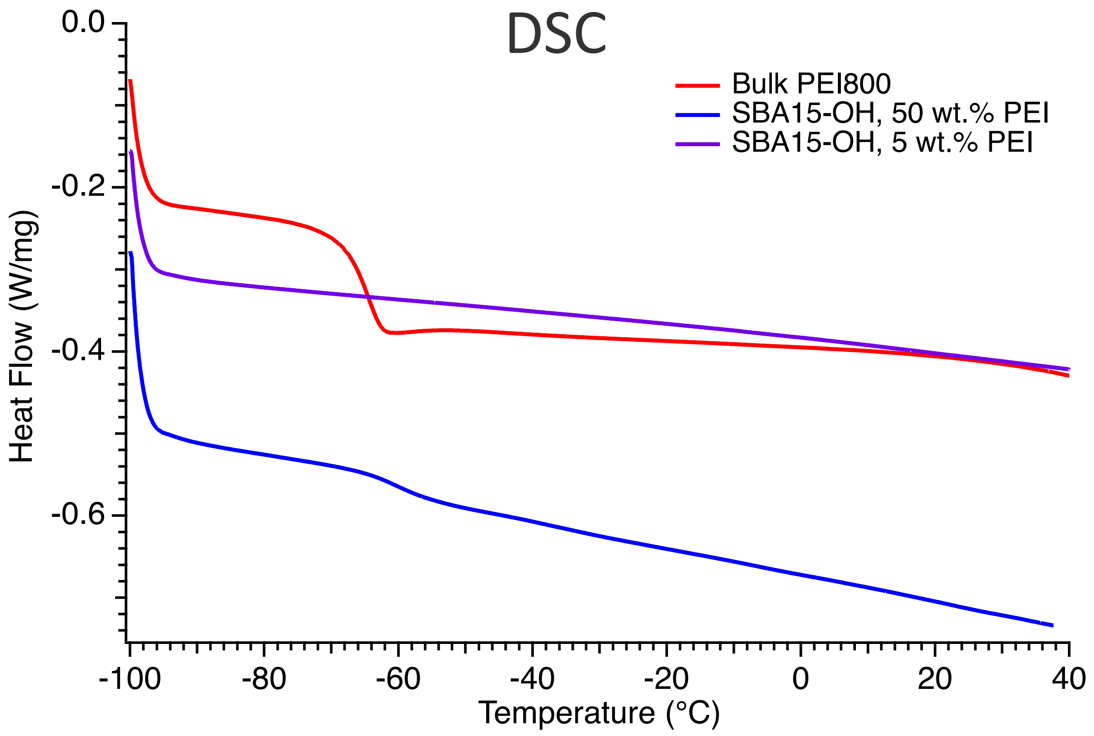
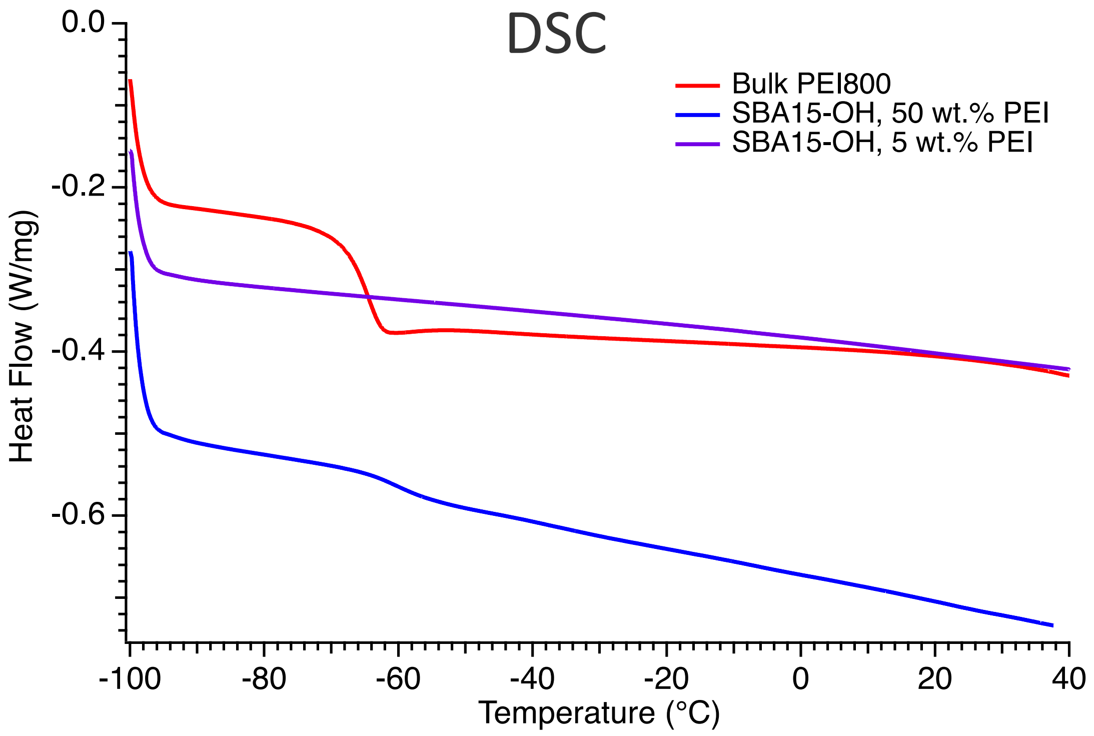
Need More Sensitive Benchtop Techniques



- Benchtop technique
- Not sufficiently sensitive for low polymer wt. fractions

Need More Sensitive Benchtop Techniques

DSC



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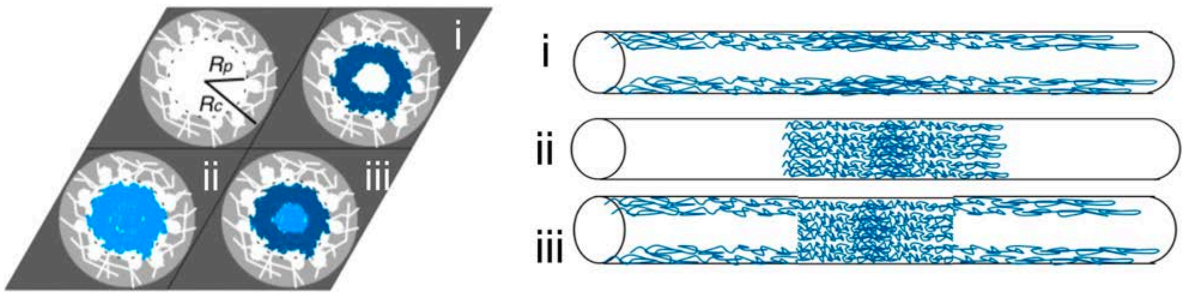
Neutron Scattering

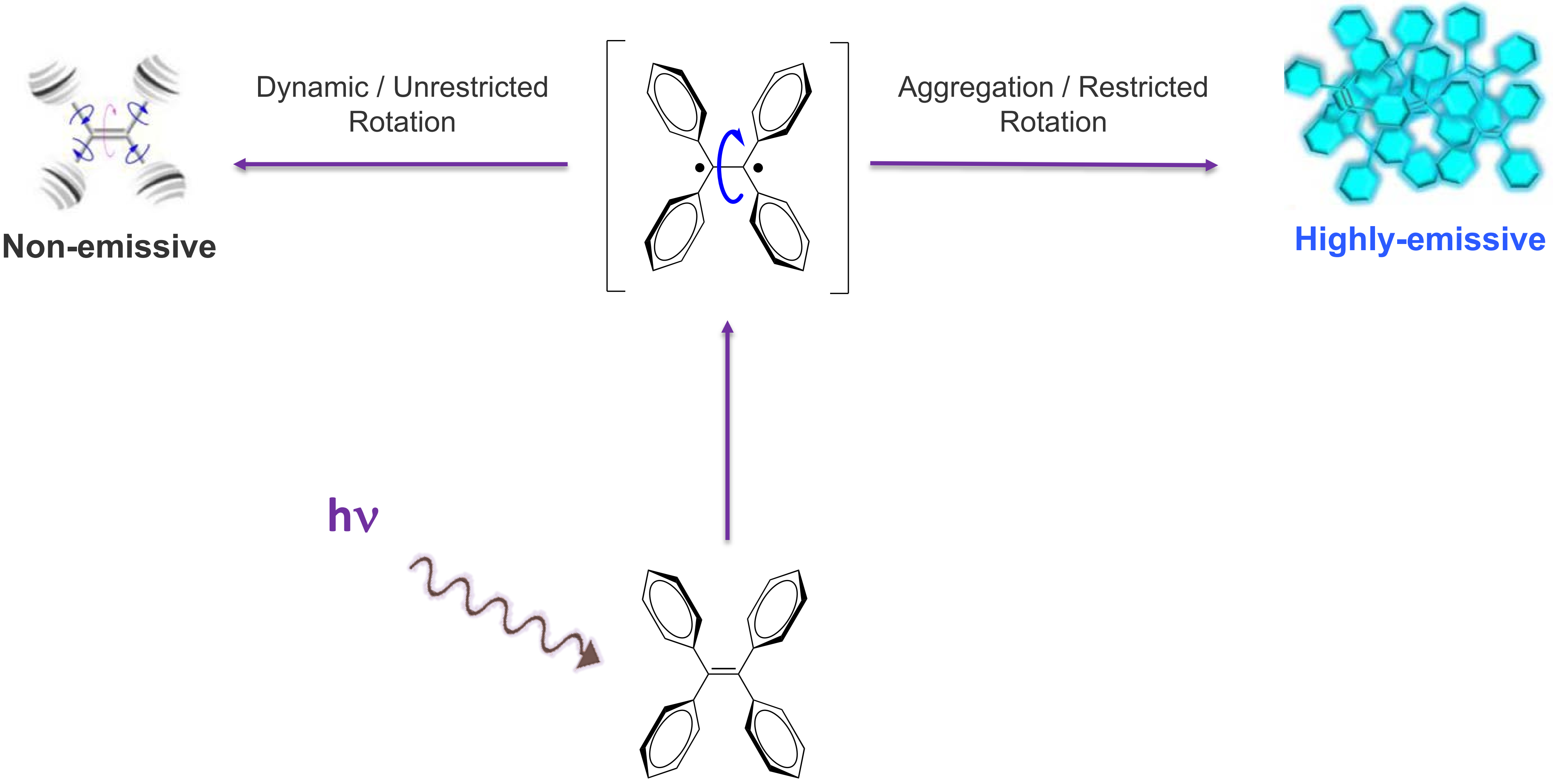


J. Am. Chem. Soc. 2015, 137, 11749

https://doi.org/10.1021/jacs.5b06823

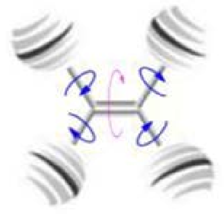
- Powerful for structure/morphology determination
- Not high-throughput

Tetraphenylethylene-Based Fluorescent Probes



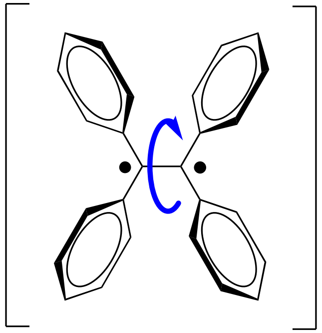
Chem. Rev. 2015, 115, 21, 11718
https://doi.org/10.1021/acs.chemrev.5b00263

Tetraphenylethylene-Based Fluorescent Probes

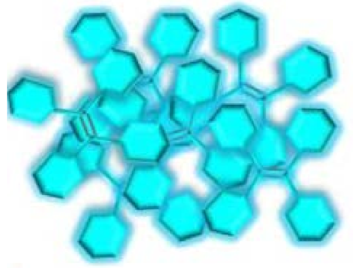


Non-emissive

Dynamic / Unrestricted Rotation

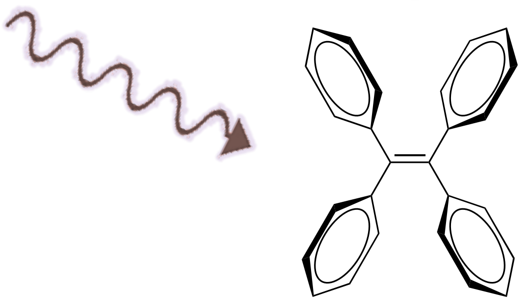


Aggregation / Restricted Rotation



Highly-emissive

hν



Chem. Rev. 2015, 115, 21, 11718
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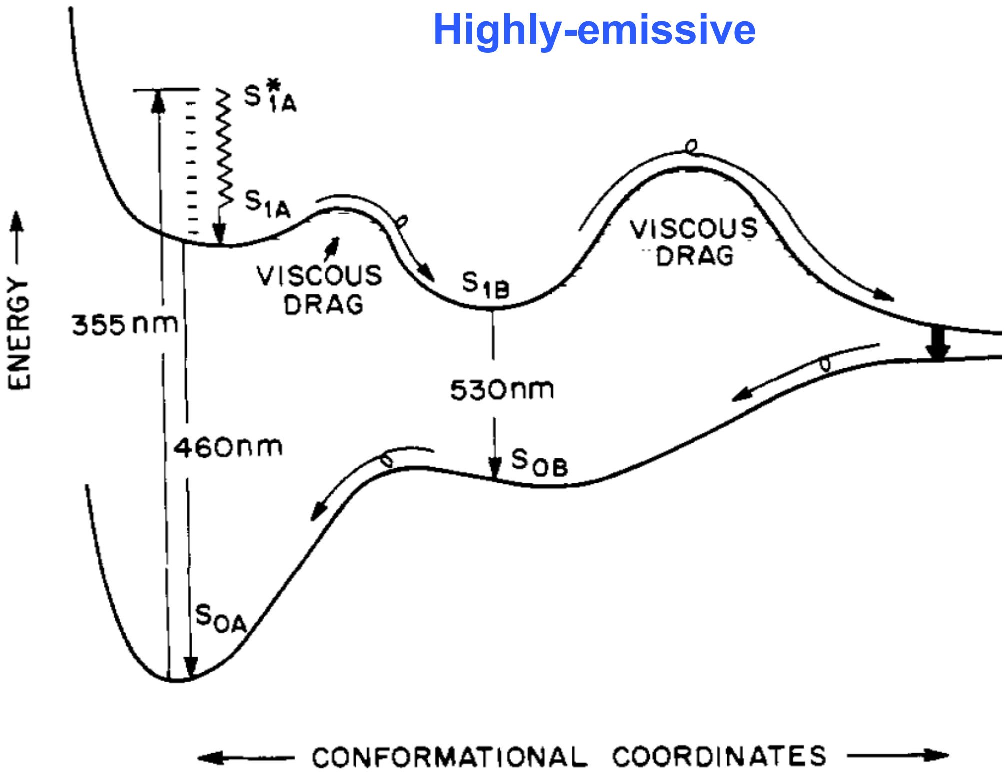
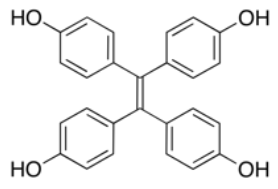
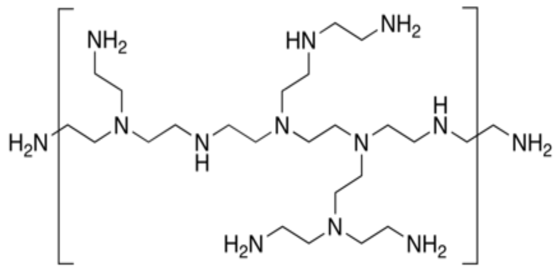


J. Am. Chem. Soc. **1981,** *103* (9), 2156
https://doi.org/10.1021/ja00399a003

Tetraphenylethylene-Based Fluorescent Probes

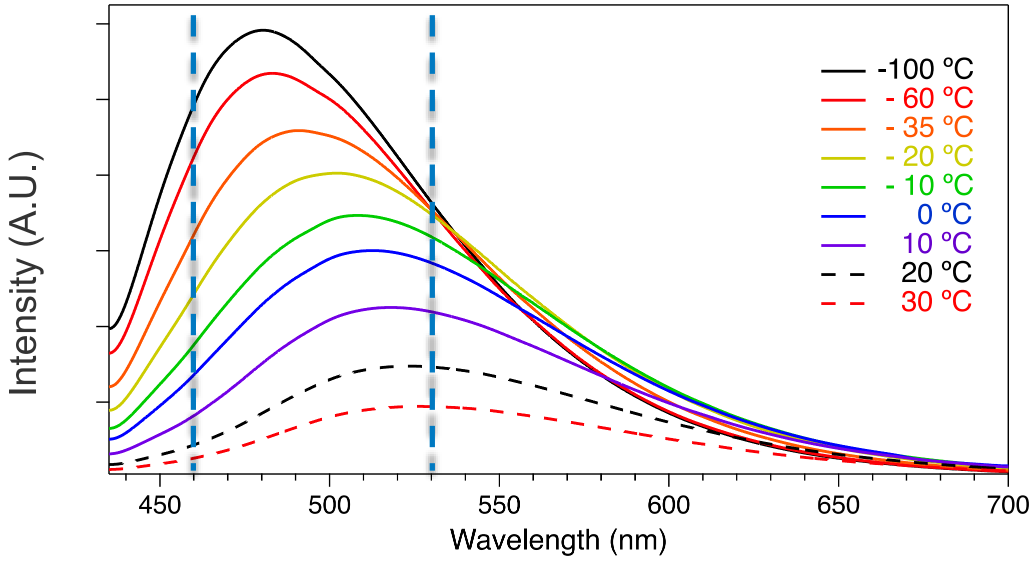


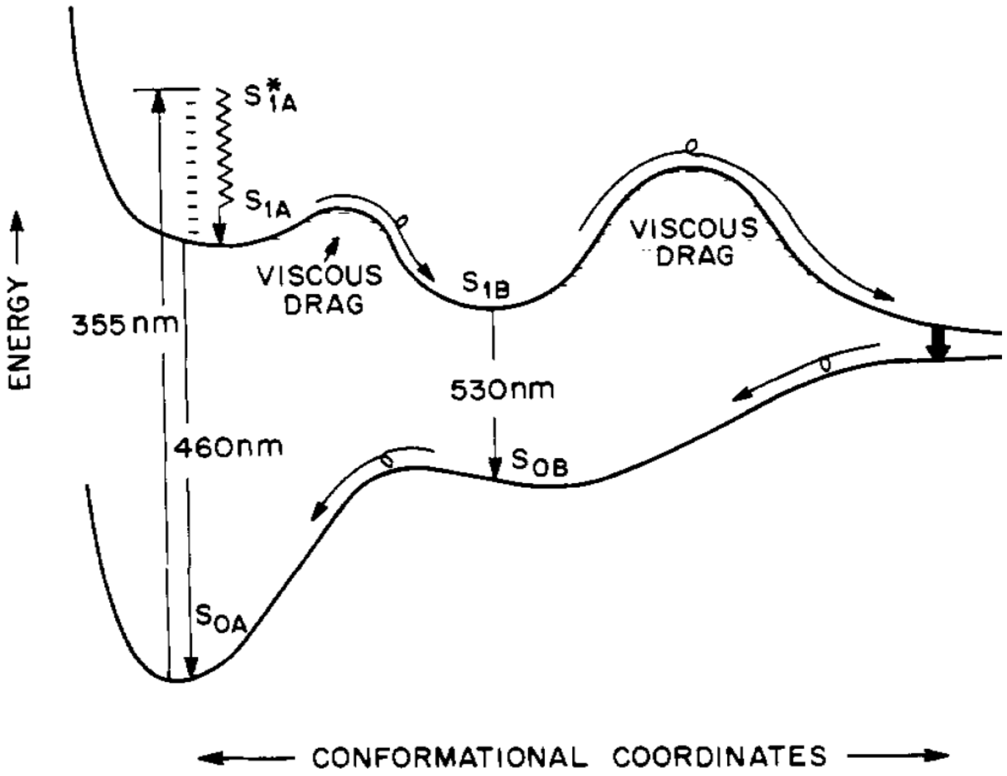
THPE



PEI_{800}

Fluorescence Spectra of PEI_{800} doped with 1 wt.% THPE





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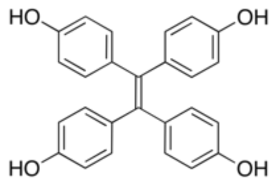
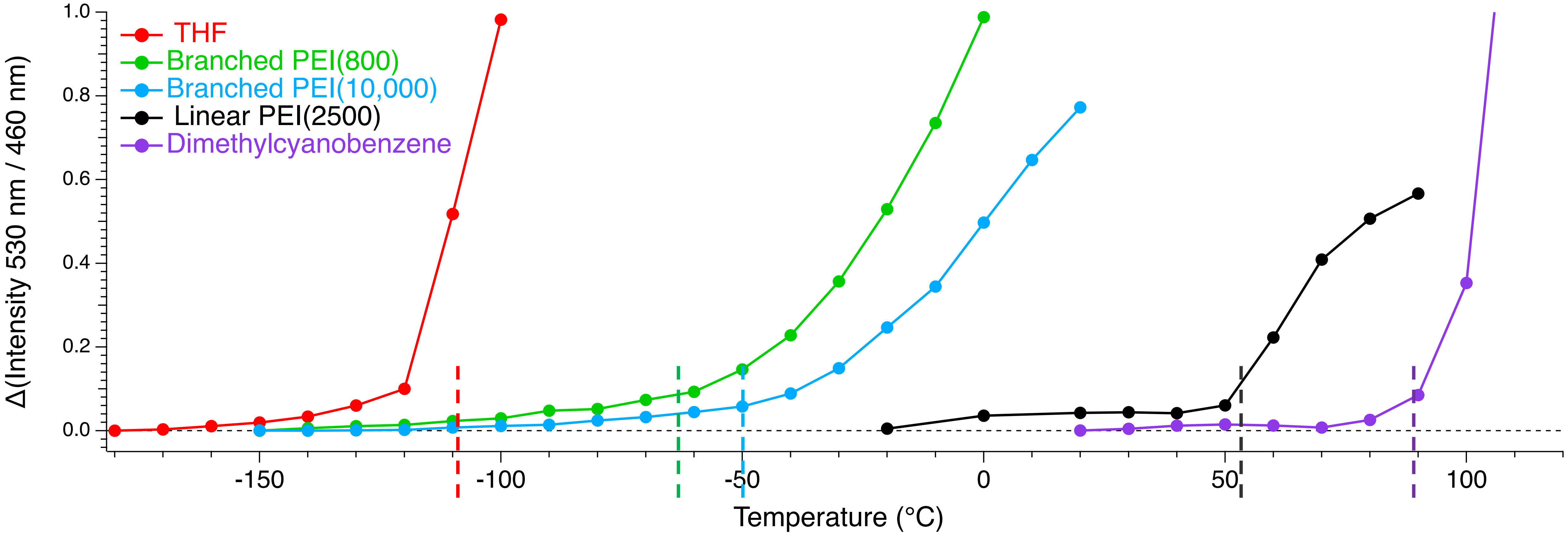
Benchmarking



THPE

- Dashed lines indicate literature T_m or T_g

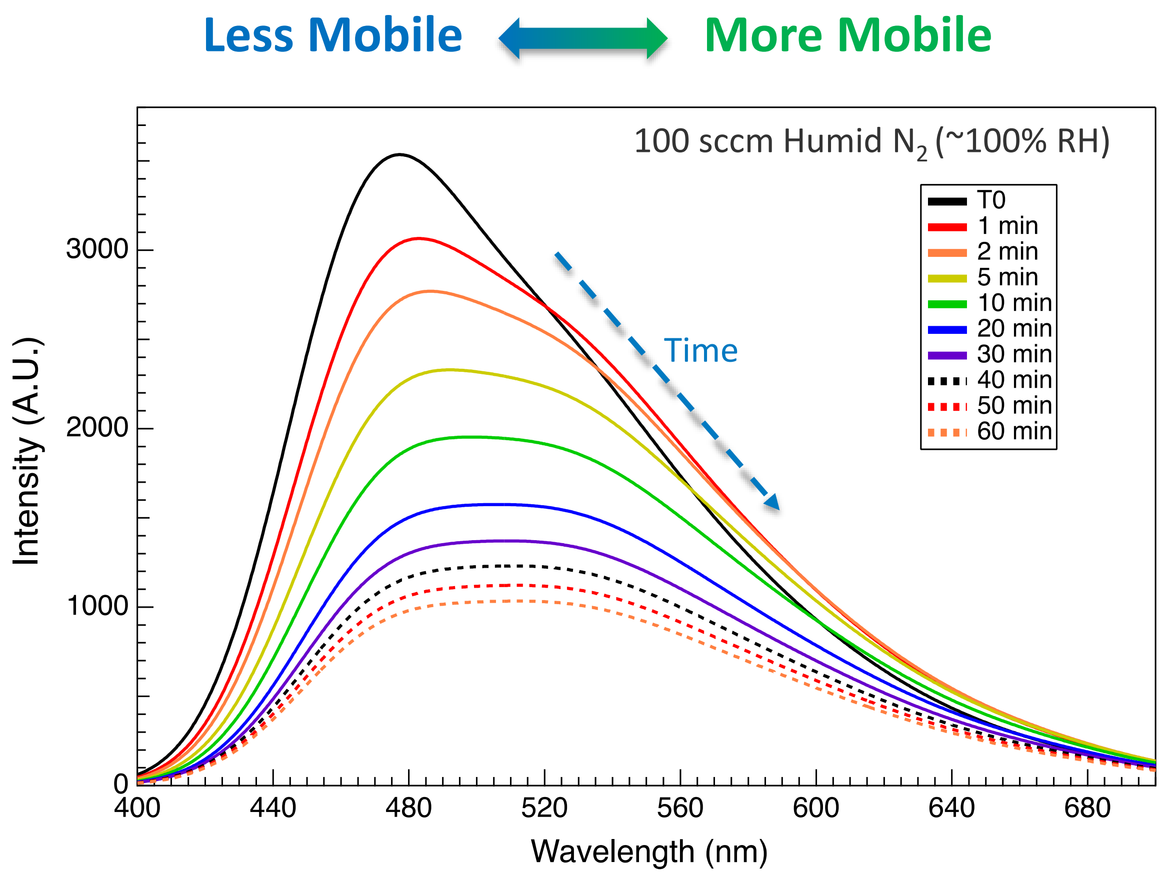


Correll, H., *et. al.*, *J. Phys. Chem. C.*, **2022**, 126, 10419.

https://doi.org/10.1021/acs.jpcc.2c01099

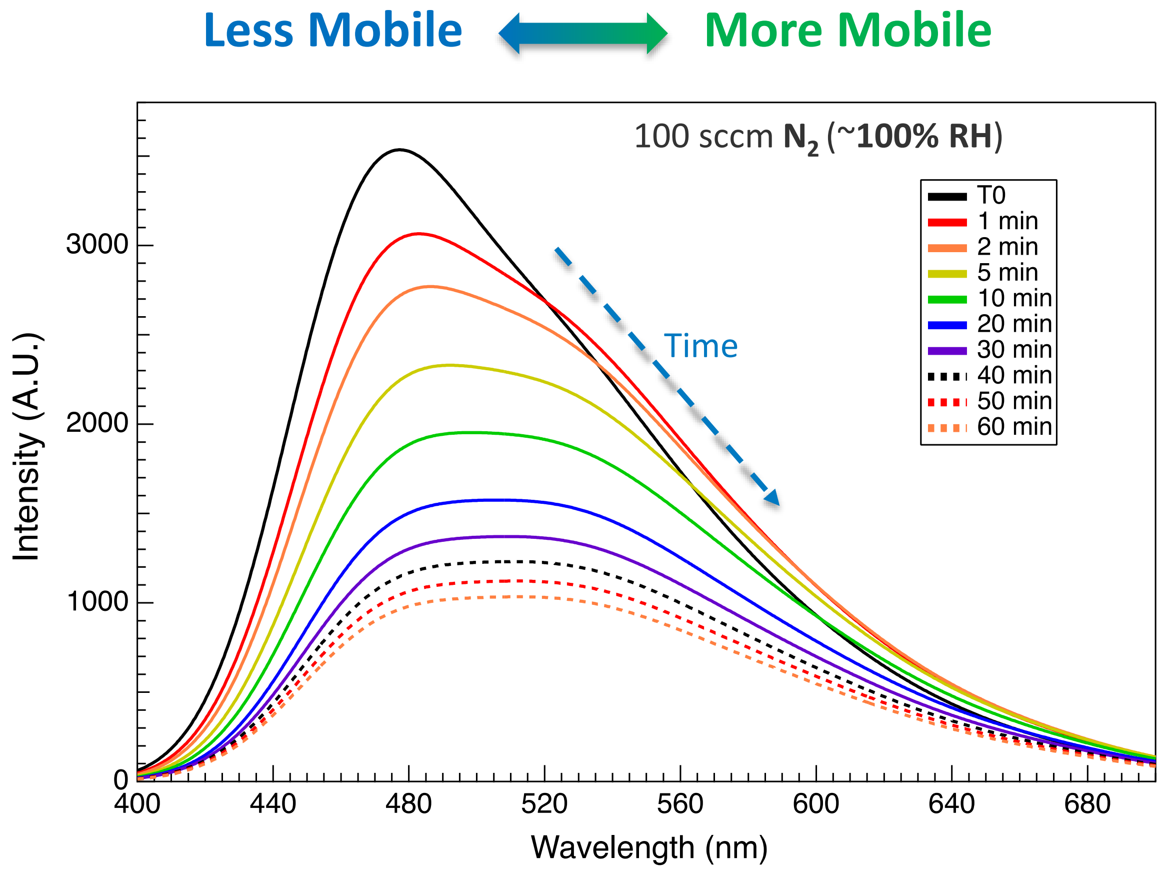
Humidity

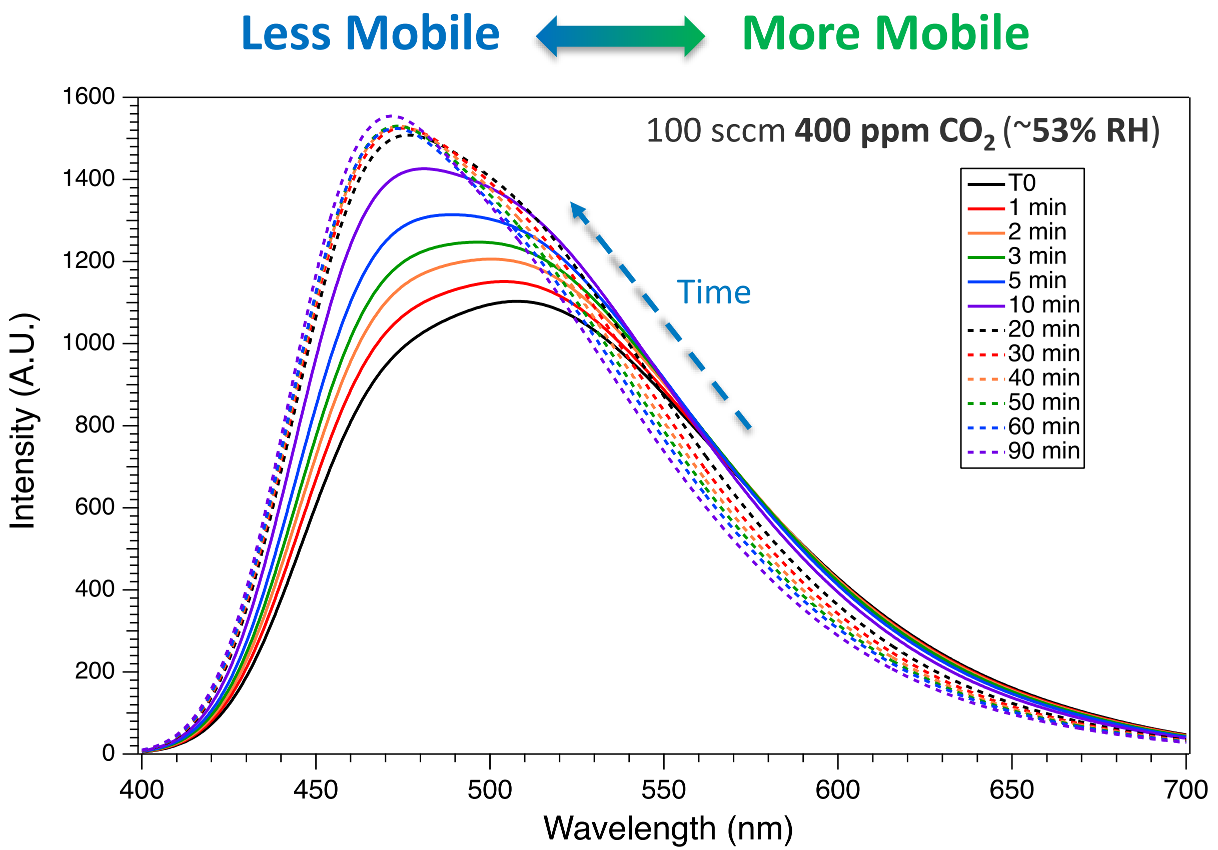
40 wt% PEI_{800} in Al_2O_3 (0.4 wt% THPE)



Humidity & CO_2

40 wt% PEI_{800} in Al_2O_3 (0.4 wt% THPE)





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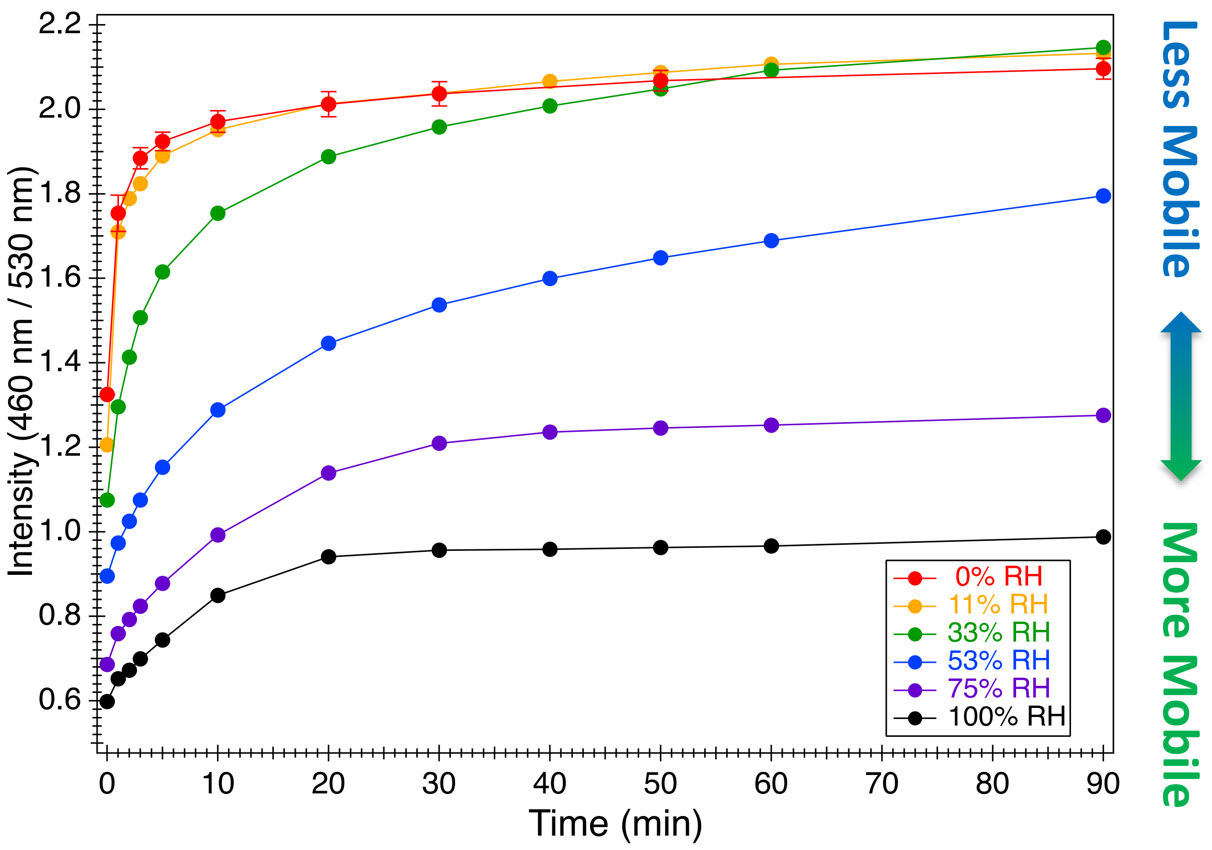

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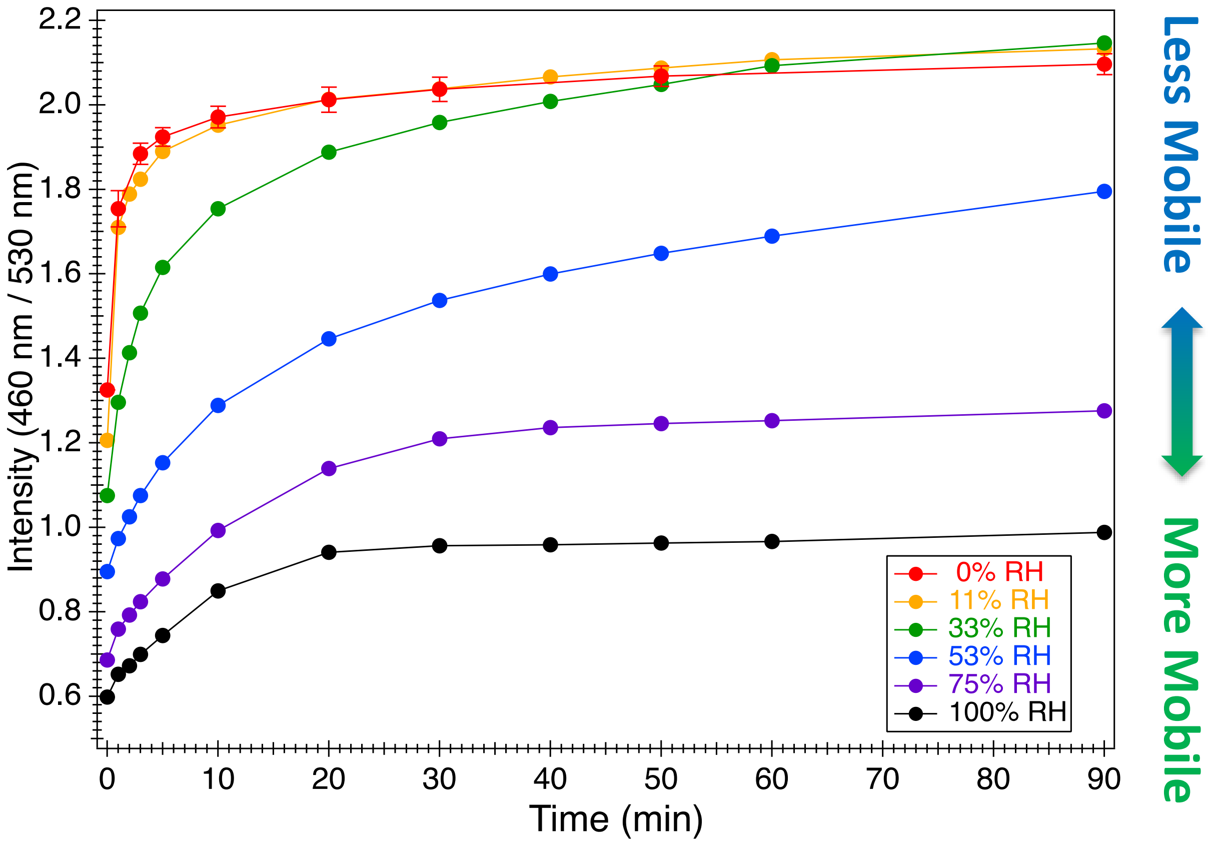
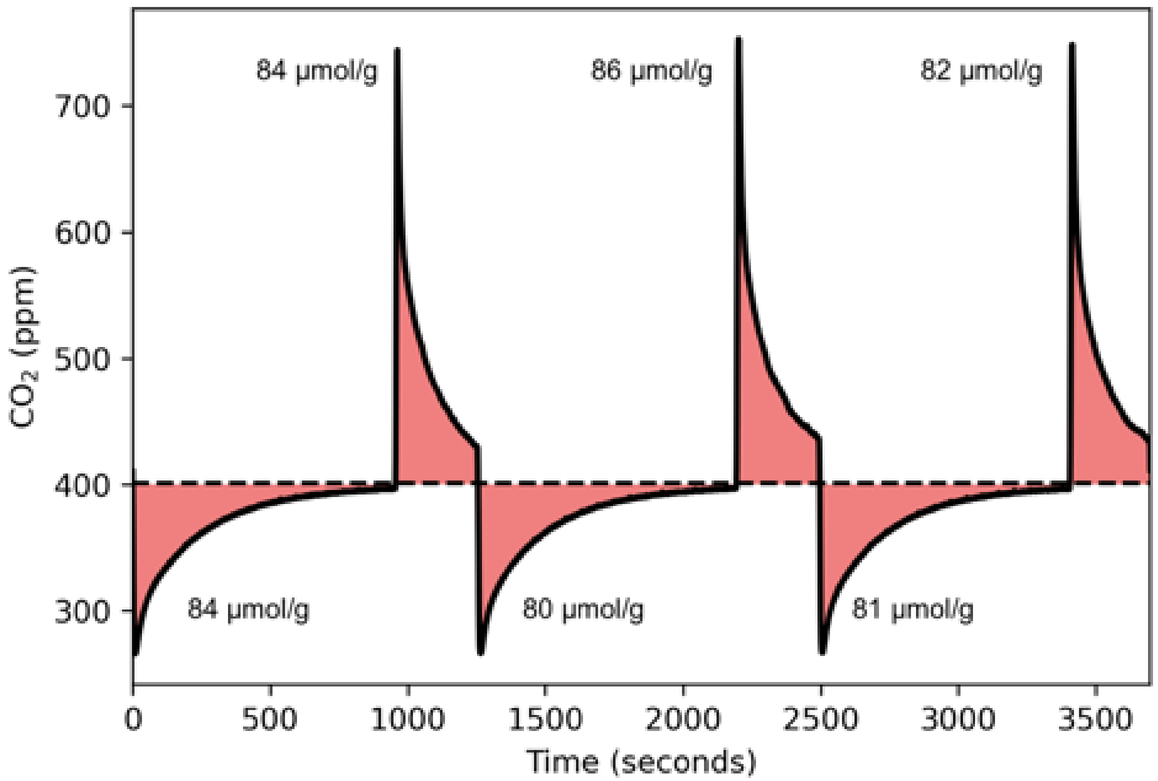


100 sccm 400 ppm CO_2



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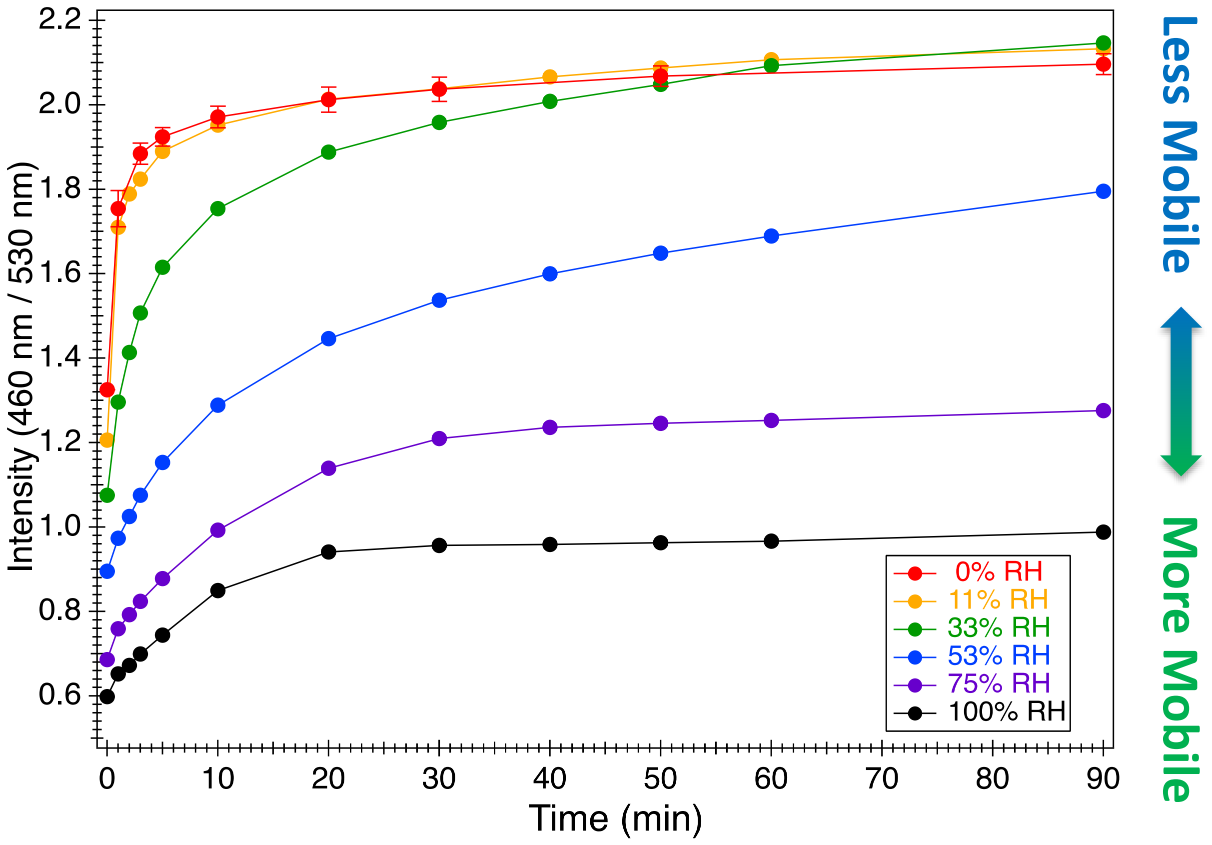

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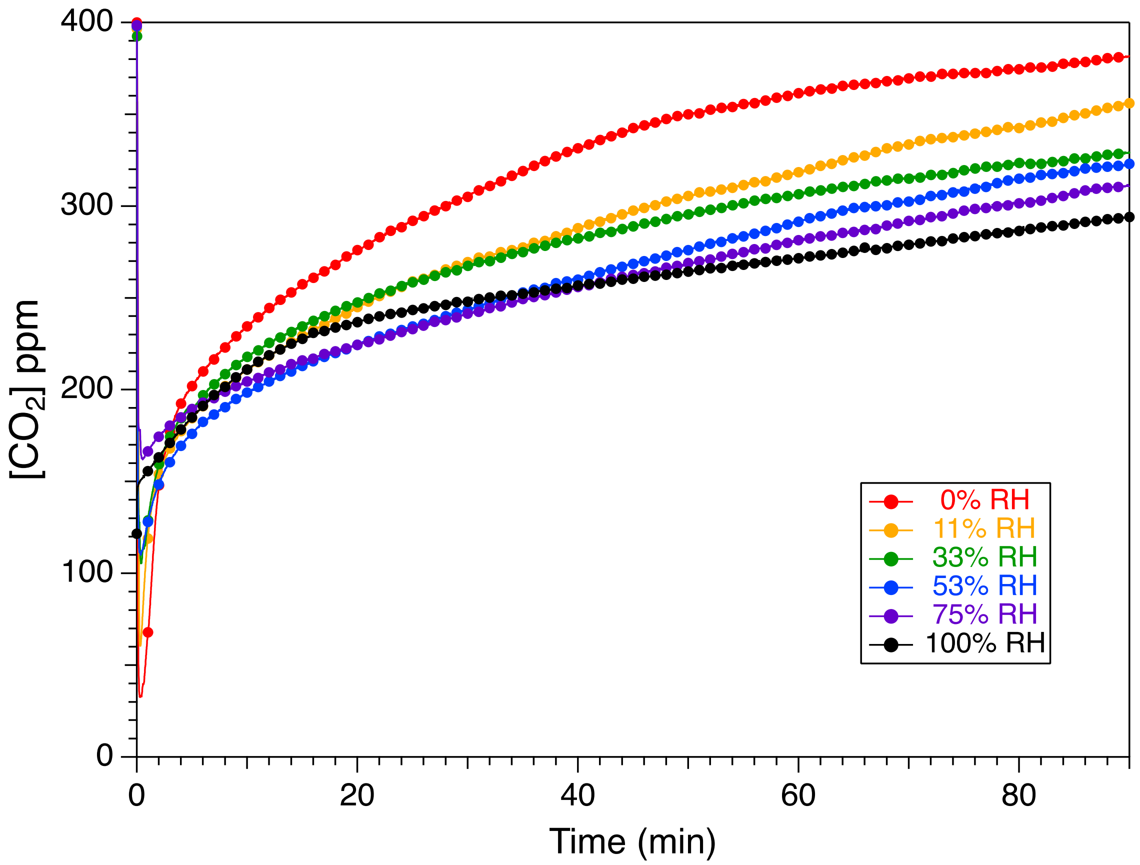

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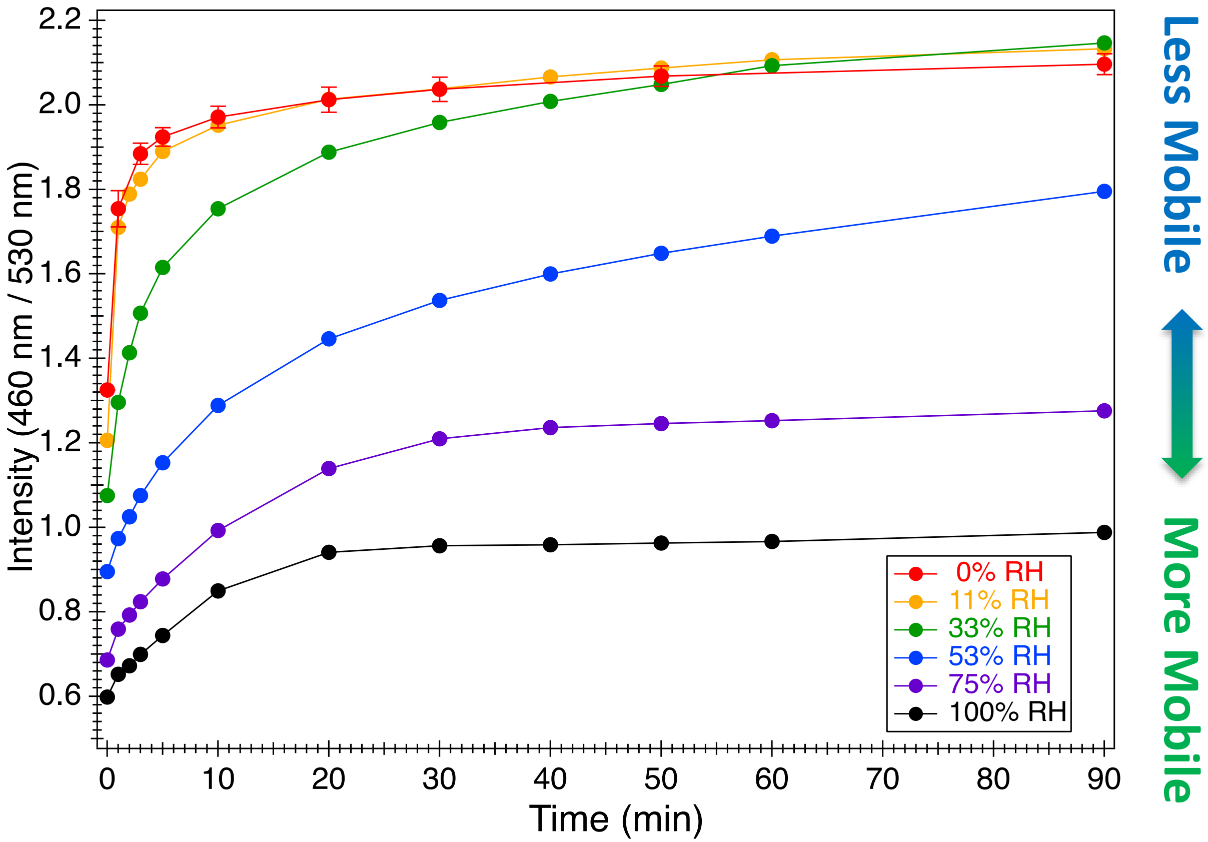
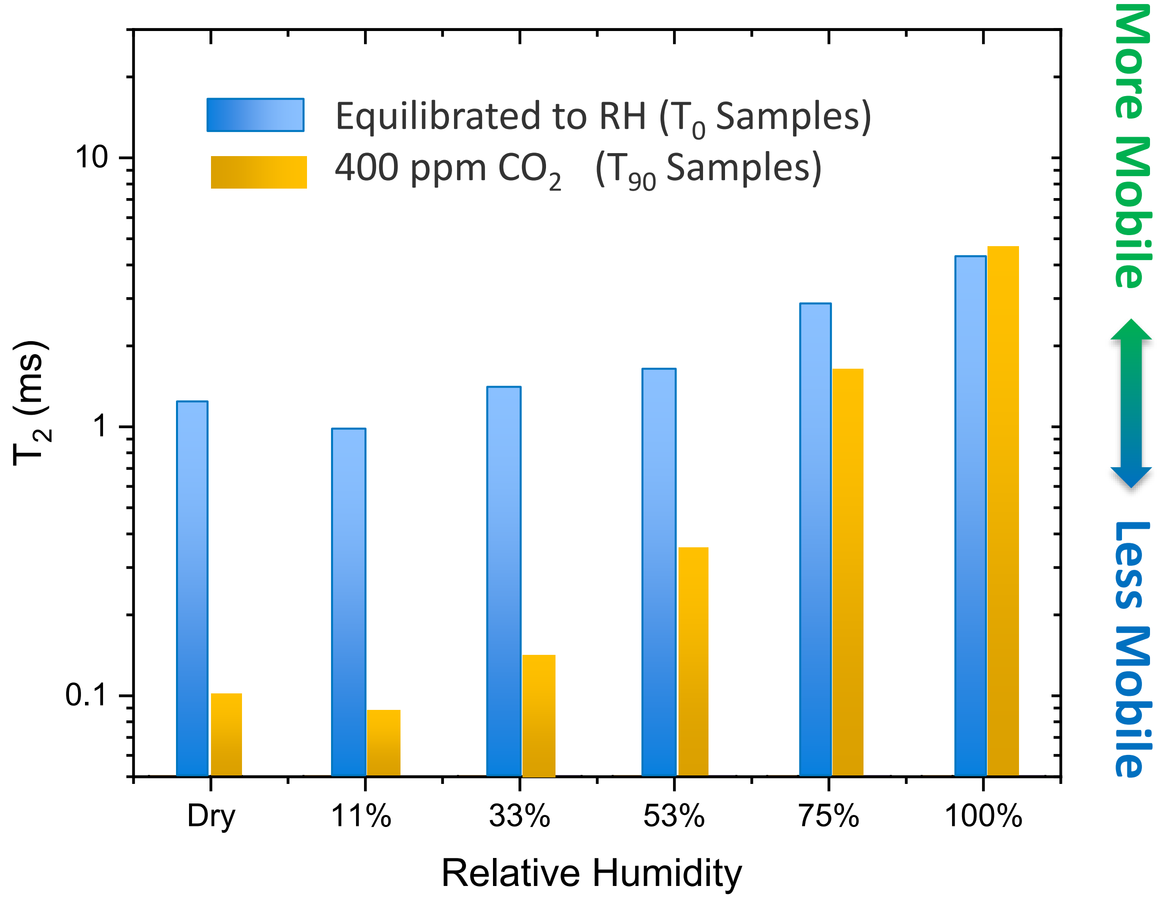
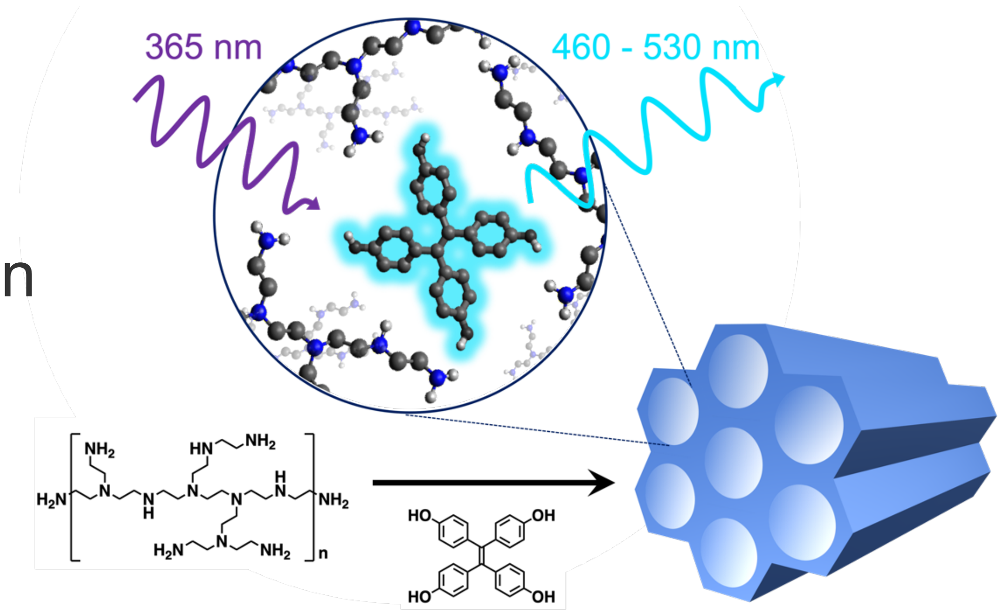




Conclusions/Future Directions

- Understanding polymer mobility is **Critical** for streamlining DAC operations
- Fluorescent probe provides sensitive benchtop analysis of mobility in confinement
- Future Directions
  - Moisture & CO_2 uptake with degradation
  - Tethered probes - spatio-temporal resolution



https://doi.org/10.1021/acs.jpcc.2c01099

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Acknowledgements

NREL	Noemi Leick
Colorado School of Mines	Glory Russell-Parks Helen Correll
LLNL	Maxwell Marple Simon Pang

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