What's New With Textiles: Understanding and Executing Plastic Layered Textiles, Coated Textiles, Fused Textiles and Polymers

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Fiber and Polymer Science Program

Footwear and Materials Innovation Summit

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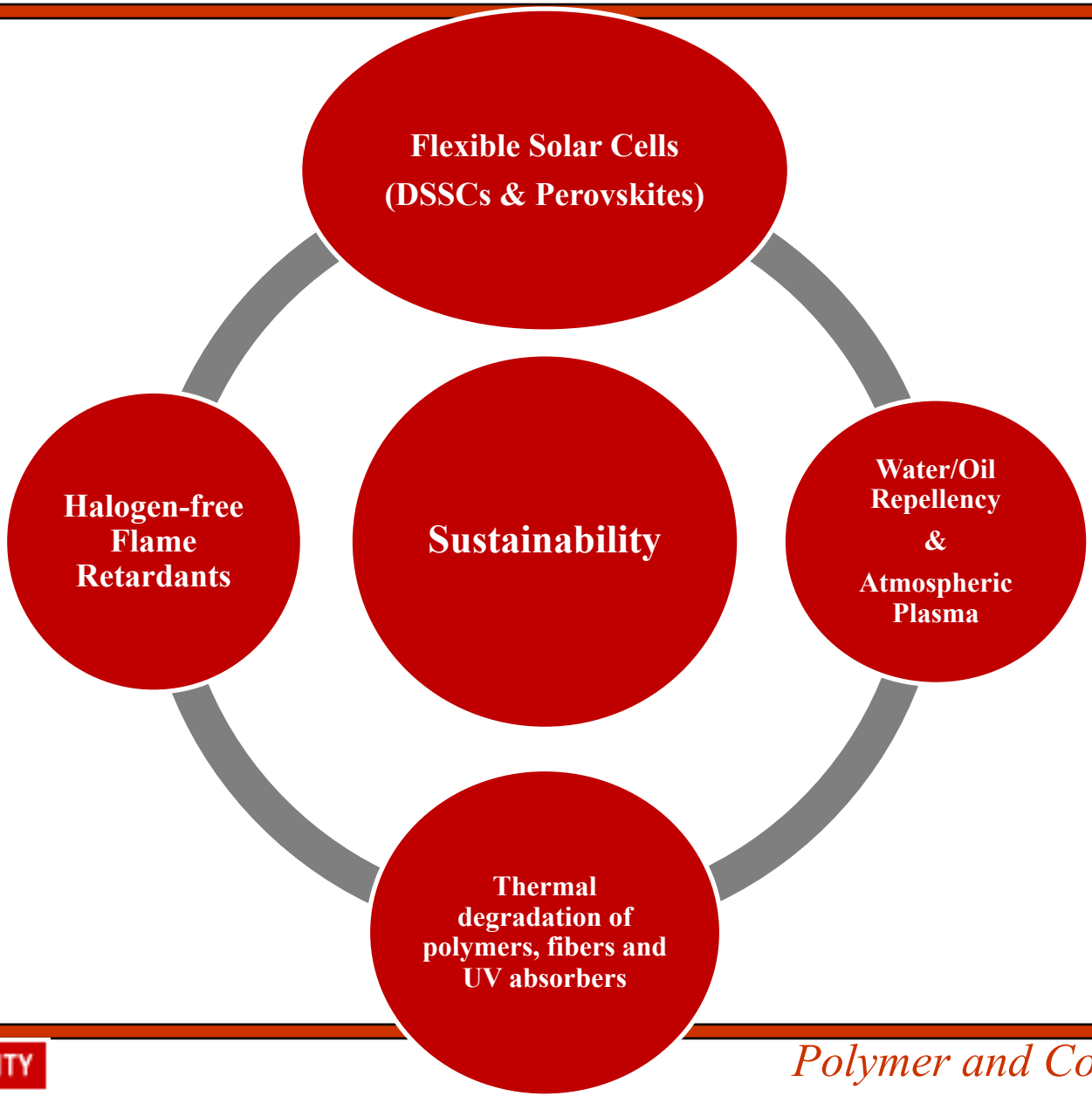
Raleigh, College of Textiles

North Carolina State University

Sustainability in El-Shafei's Group

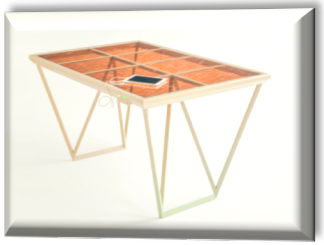


College of Textiles-Centennial Campus

El-Shafei's Research Group

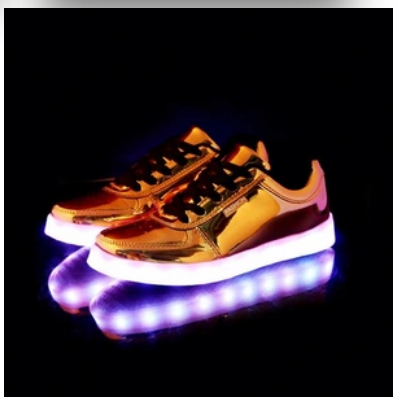
El-Shafei's Research Group-Recovering from Snow

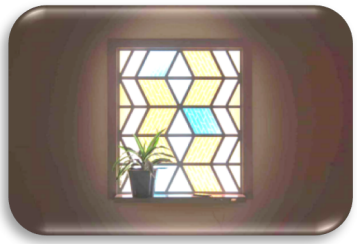
Flexible Dye-Sensitized Solar Cell (DSSC)



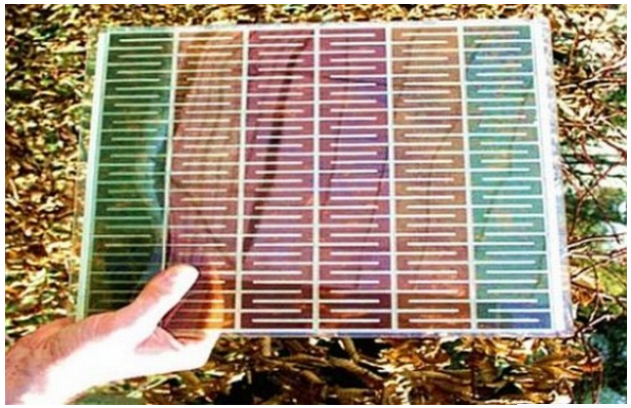
Advantages:

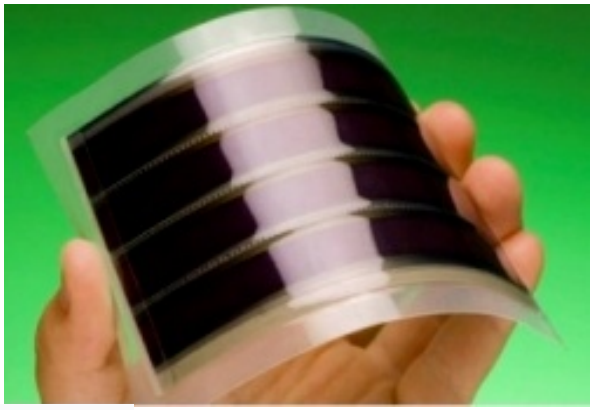
1) Low production cost;
2) Multi-color design;
3) Transparency;
4) Flexibility in designing;
5) Superior performance in diffuse light;
    1) Works great in a rainy or cloudy day
        - Can be integrated into a shoe to charge your cellphone (wireless)
6) Molecular design opportunities.

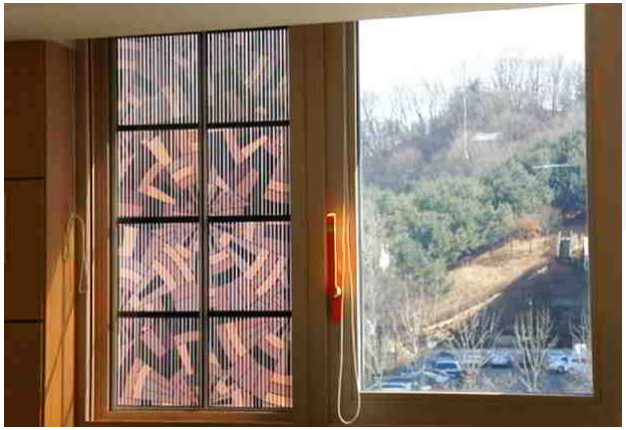




DSSCs





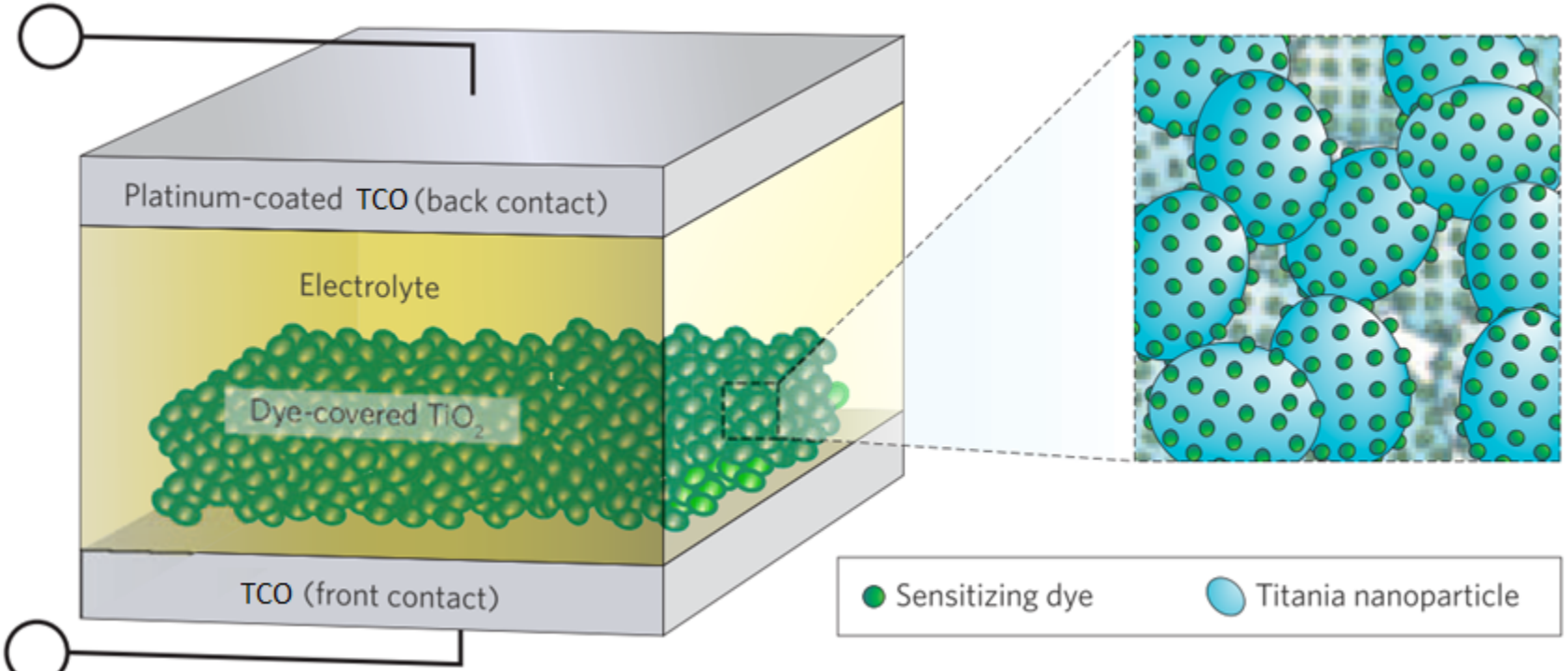


Leaf-shaped DSSCs

Facade- Dyesol Ltd

Components of DSSC

1) TCO substrate;
2) Semiconductor;
3) Dye sensitizer;
4) Electrolyte;
5) Counter electrode.

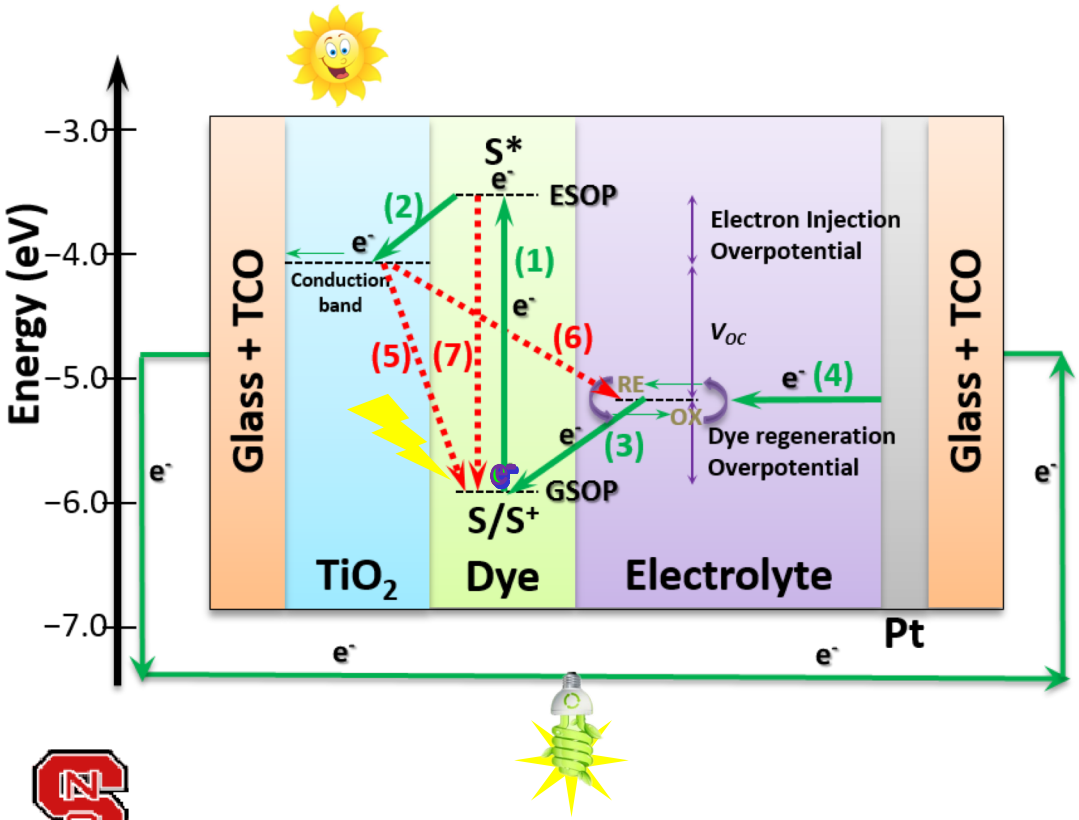


McGehee, M. D. *et al*. *Nat. Photonics* **2012,** *6*, 162-169.

Operation Principle of DSSCs

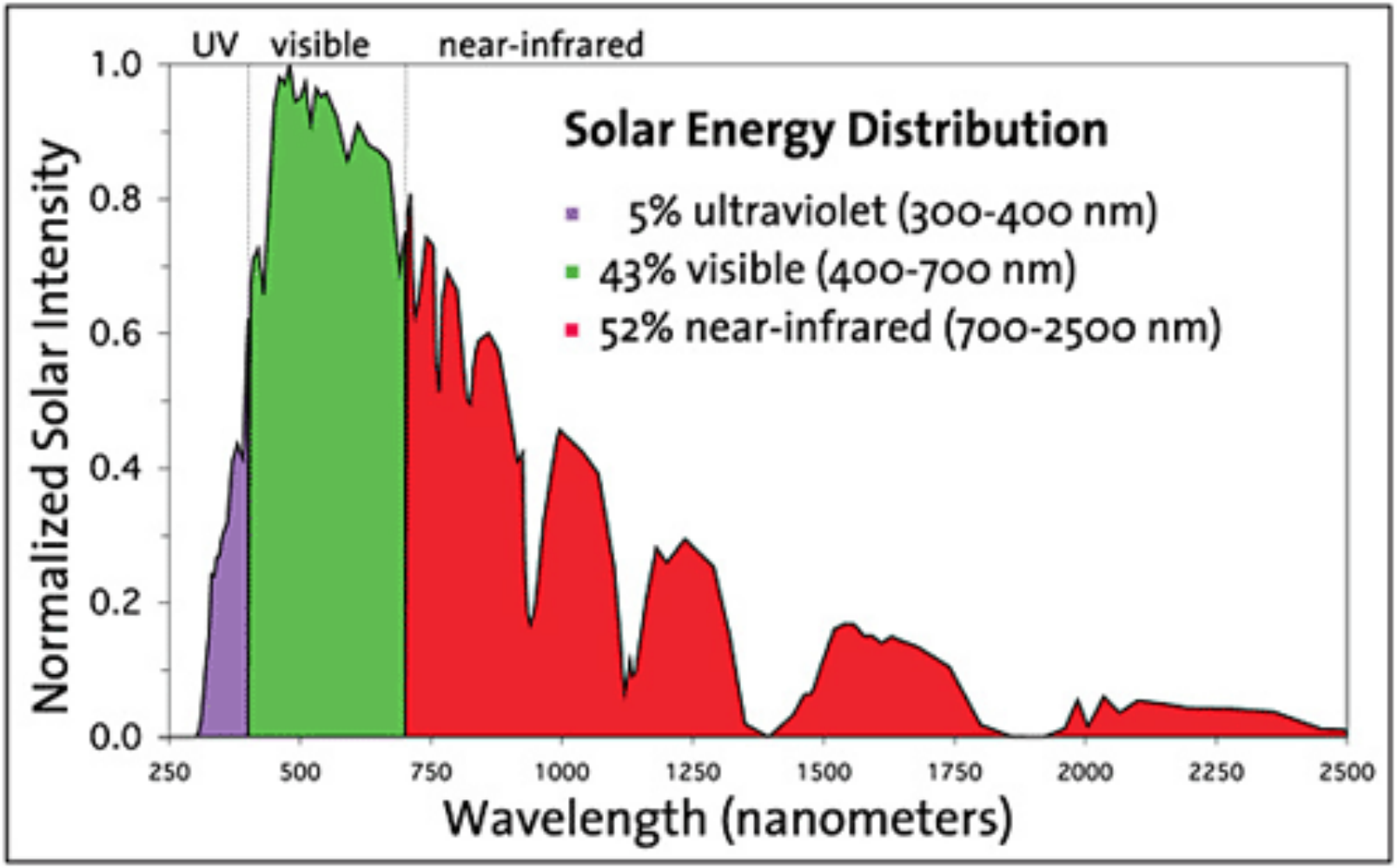
To absorb light, separate charge and collect charge

Natural photosynthesis



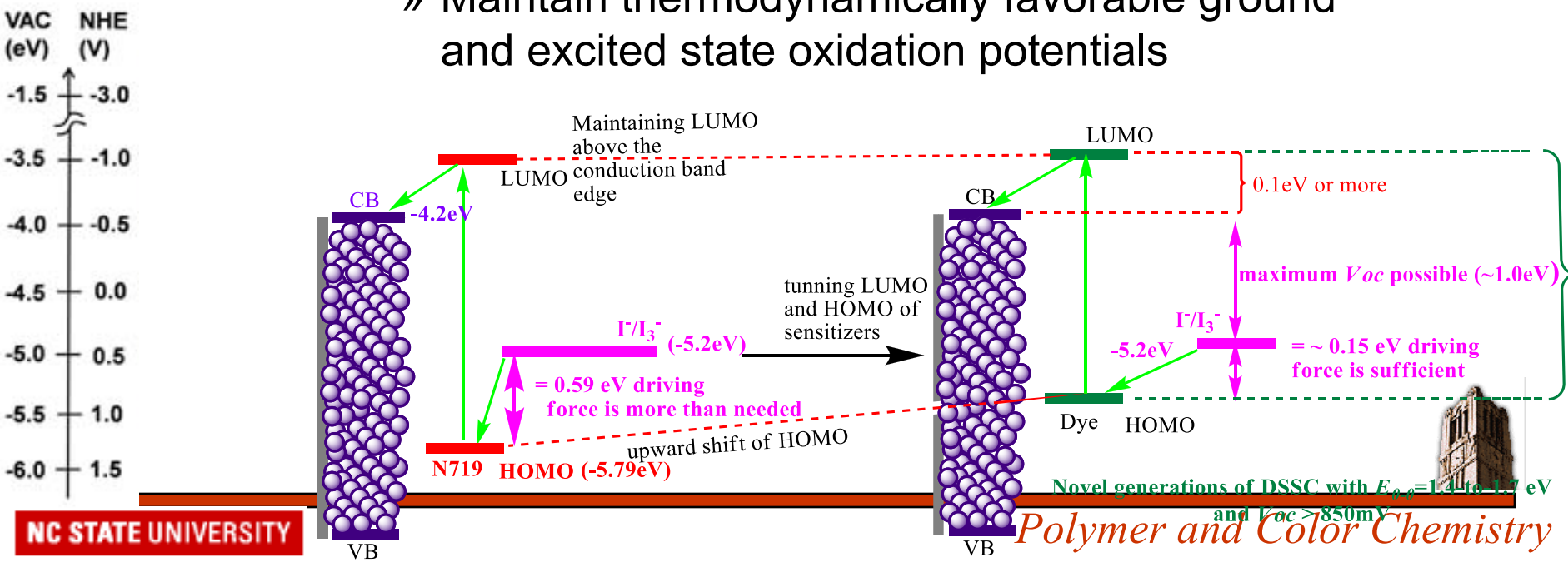
1) Photoexcitation;
2) Electron injection;
3) Dye regeneration;
4) Regeneration of redox couple;
5) Electron recombination with oxidized dye;
6) Electron recombination with redox couple (dark current);
7) Electron decay.

Solar Spectrum

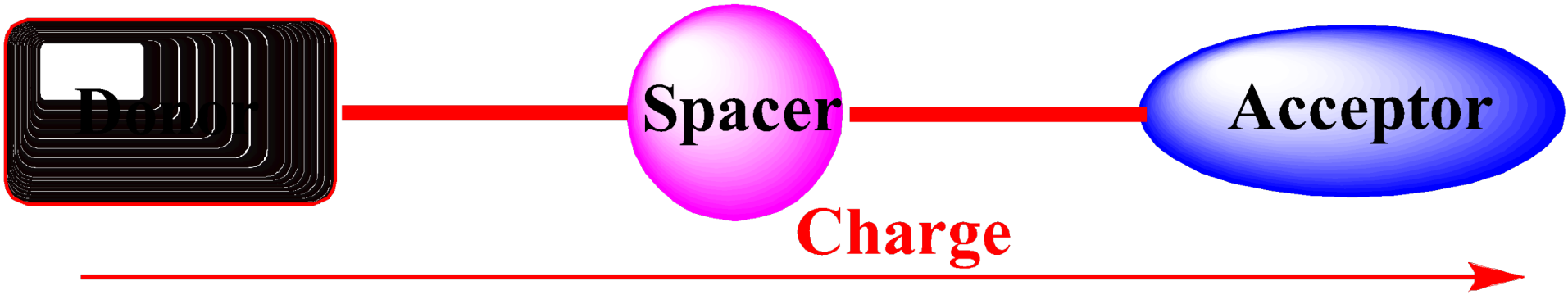


Strategy

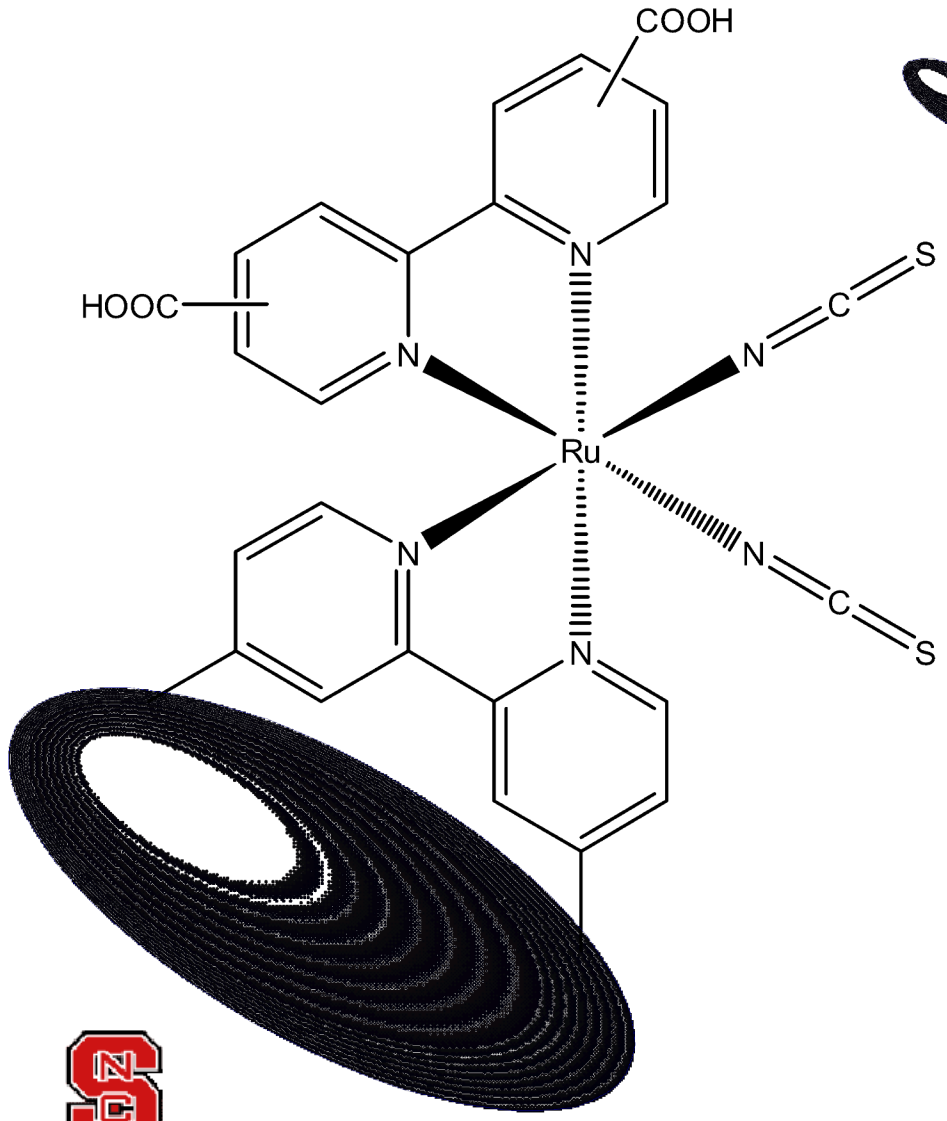
- Enhance the optical molar absorptivity in the visible and NIR regions compared to the benchmark N719
  - Furnish more red shifted-better light harvesting efficiency across a wider range of solar spectrum
    - » Narrow HOMO-LUMO gap
    - » Maintain thermodynamically favorable ground and excited state oxidation potentials



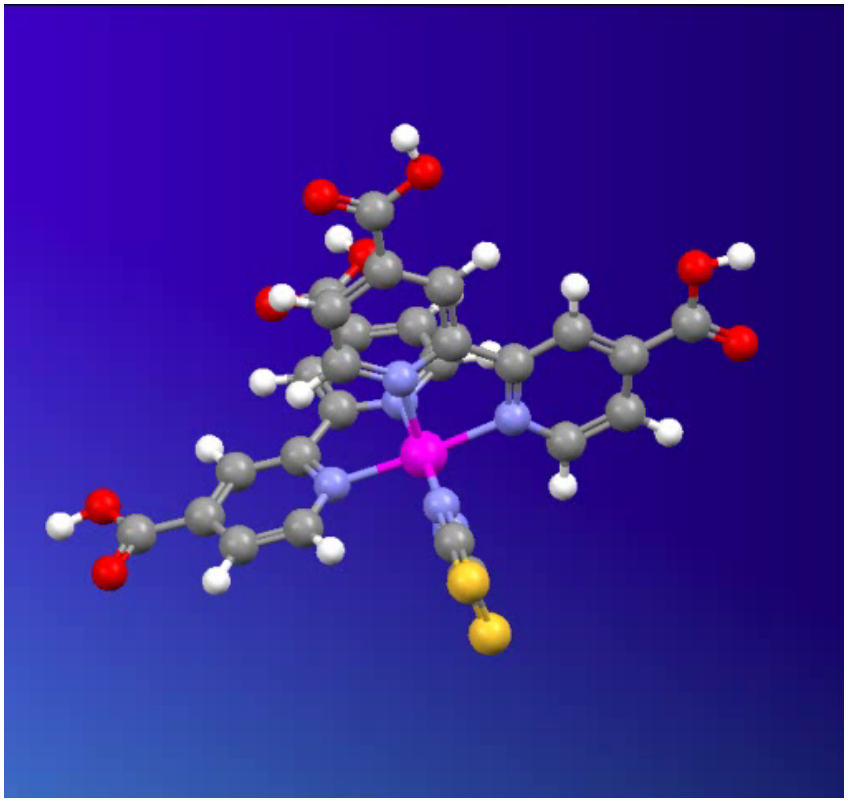
Molecular Engineering of High Efficiency Photosensitizers for Dye-sensitized Solar Cells



Structure Modulations of Ancillary Ligands

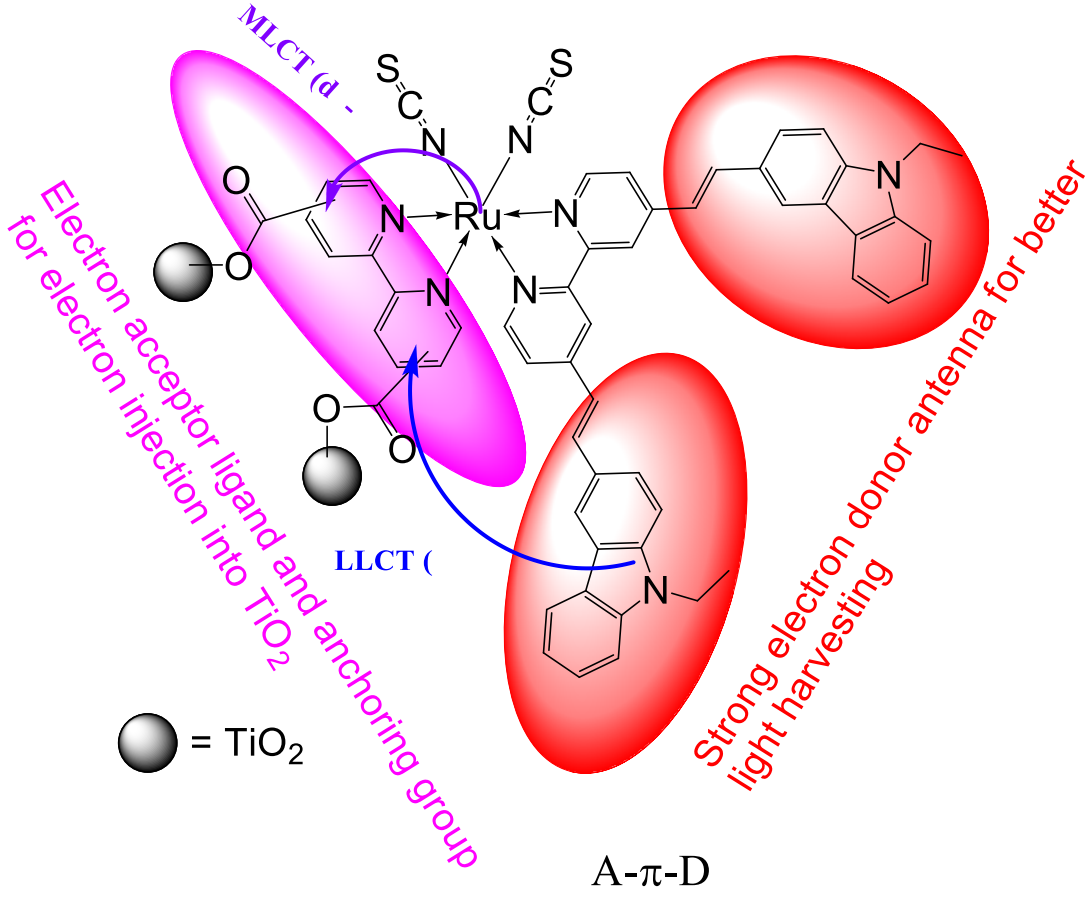


= Ancillary ligand



Carbazole Antenna

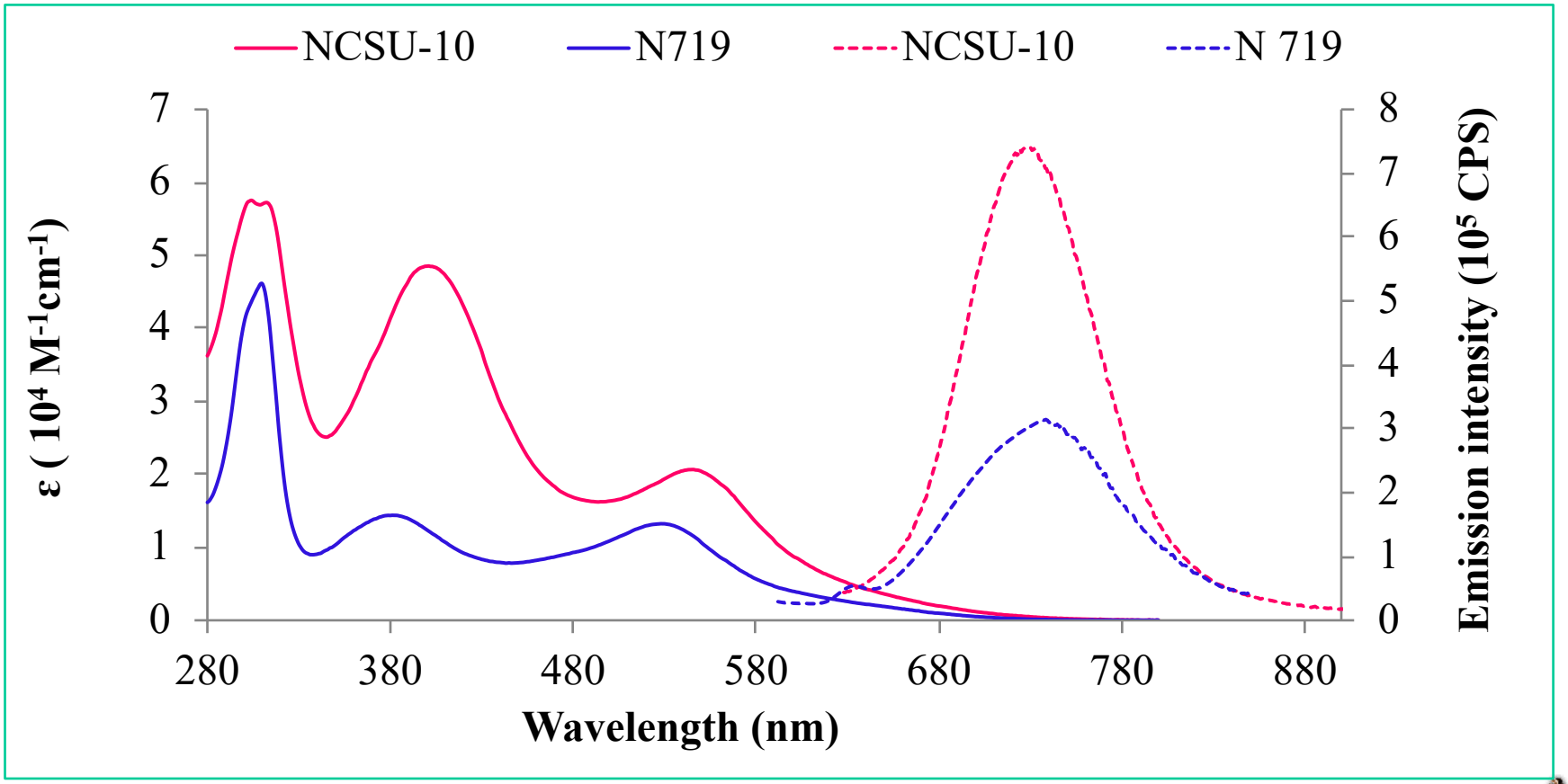
- NCSU-10



NCSU-10	4,4'-COOH
NCSU-10'	5,5'-COOH

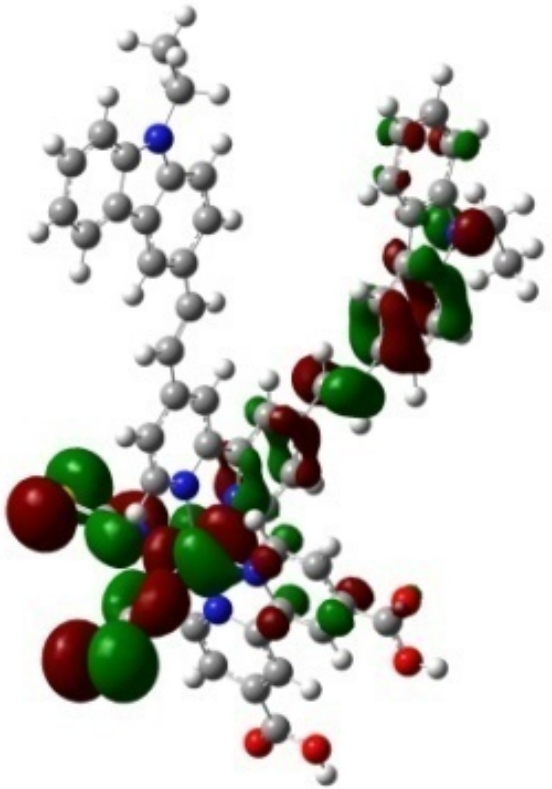
NCSU-10 vs N719

- UV-Vis absorption and emission spectra

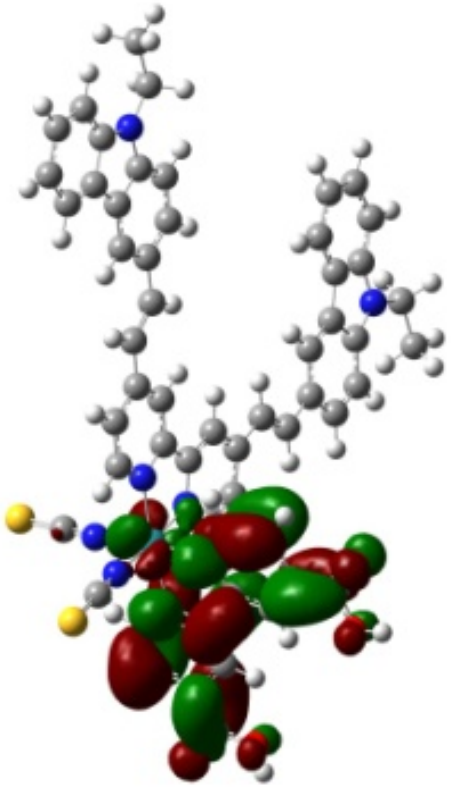


Carbazole Antenna: NCSU-10

- HOMO and LUMO delocalization (TD-DFT)



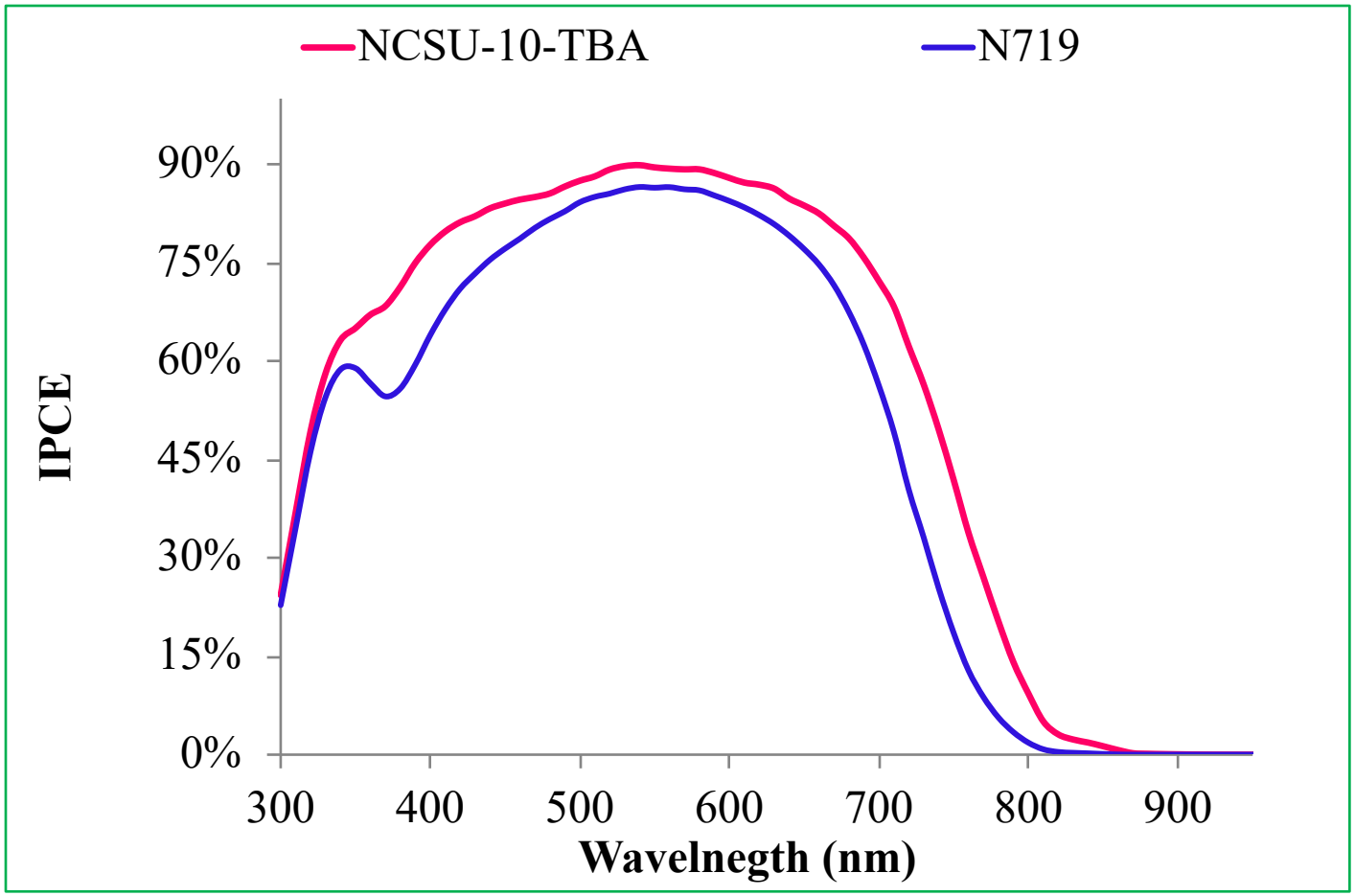
HOMO (NCSU-10)



LUMO (NCSU-10)

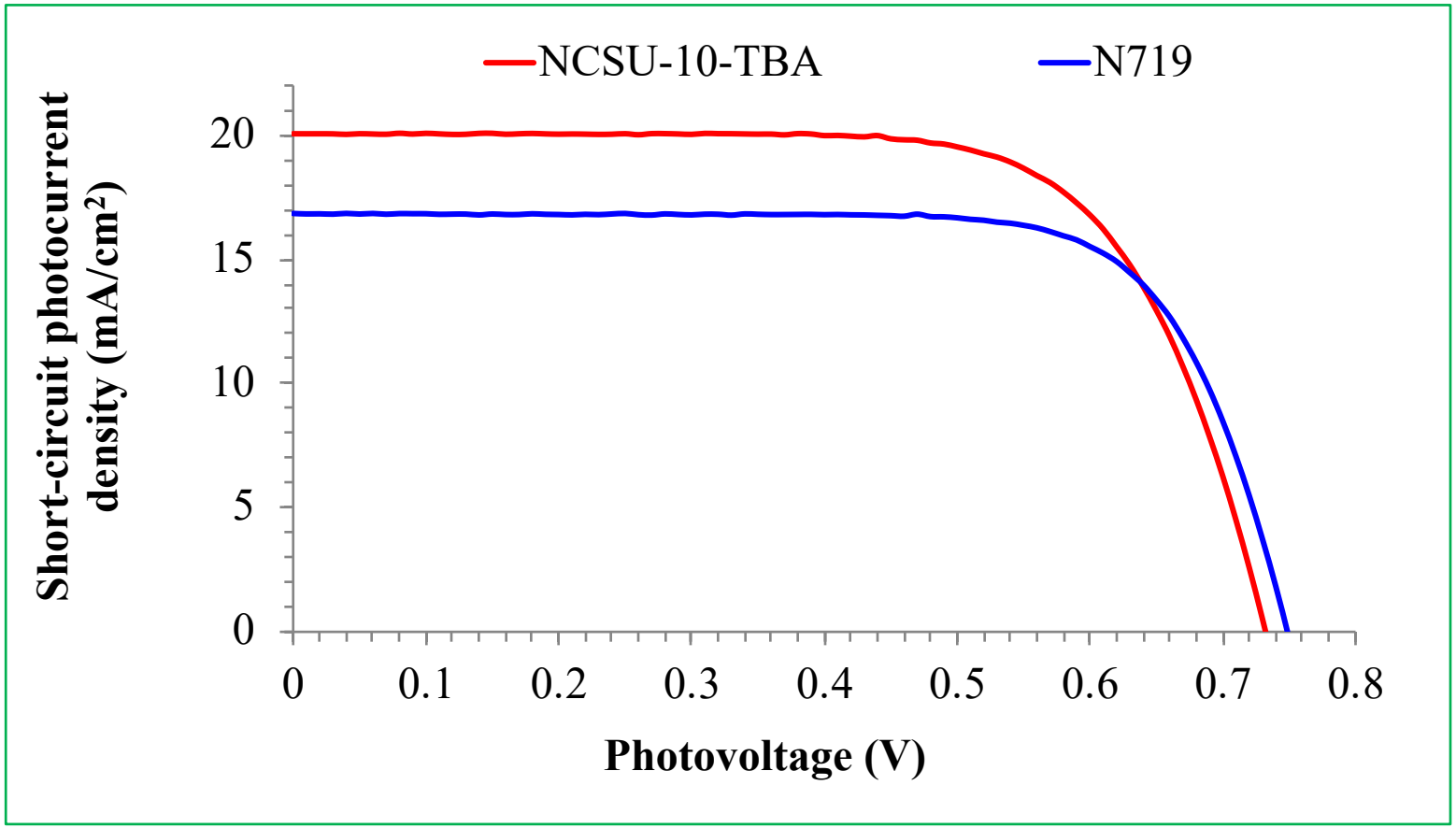
Carbazole Antenna: NCSU-10

- Incident Photon to Current Efficiency Conversion (IPCE)



Carbazole Antenna: NCSU-10

- I-V characteristics



El-Shafei et al. publications

- *J. Mater. Chem.* (22) , 2012 (24048-24056)
  - NCSU-10 achieved 10.3% efficiency compared to 9.3% for N719
- *J. Mater. Chem. A,, 2012, DOI: 10.1039/C3TA12748F*)
  - Cyclic electron donor achieved better photovoltaic performance (cyclic) achieved 9.91% compared to 9.3% for N719
- ***Progress in Photovoltaics: Research and Applications, 2013, DOI: 10.1002/pip.2349.***
- ***Physical Chemistry Chemical Physics, 2012, DOI:10.1039/C3CP51260F*); MH11 (pyrene) achieved 10.06% compared to 9.3% of N719**
- ***Advanced Energy Materials*, *2014, DOI:10.1002/aenm.201400085***
  - **High Efficiency NIR dyes (*translucent solar cells*)**

Co-sensitization

- Praveen Naik, Rui Su, Mohamed Ramadan Ahmed Elmorsy, Ahmed El-Shafei, Airody Adhikari, New carbazole based dyes as effective co-sensitizers for DSSCs sensitized with Ruthenium (II) complex (NCSU-10), *Journal of Energy Chemistry*, 2018, DOI: https://doi.org/10.1016/j.jechem.2017.12.013

Co-sensitization

- Praveen Naik, Rui Su, Mohamed R. Elmorsy, Ahmed El-Shafei, Airody Adhikari, Investigation of new carbazole based metal-free dyes as active photo-sensitizers/co-sensitizers for DSSCs, *Dyes and Pigments*, *DOI: 10.1016/j.dyepig.2017.09.068*

Multifunctional Materials

- To Avoid shoes odor, enhances water/oil repellency and flame retardancy
  - Halogen-free flame retardant chemistry
    - No melting
    - No dripping
    - Self extinguishable
    - No toxic smoke
  - Fluid repellency and antimicrobial

Universal Halogen-Free Flame Retardants

Brian: Cotton

Stacy: Nonwovens PET and PP

Why Do We Care About This Research?

- In 2013 the US saw $11.5 billion in property damage
- 3,240 deaths from fire
- 15% of the 1.24 million total fires in 2013 were highway vehicles
  - 300 resultant deaths
- Between 2005-2009 an average of 7,040 home fires per year began with upholstered furniture

Why Do We Care About This Research?

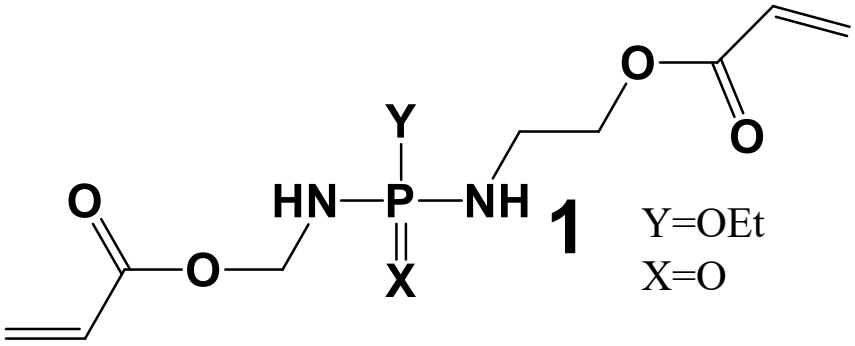
- **Halogenated FRs**
  - Very effective in vapor phase
    - Negative effects
      - Toxic
      - Bioaccumulative
      - Persistent
      - Endocrine Disruptive
  - **Phosphorus FRs operate in the condensed phase**
    - Char prevents flame from reaching fiber
    - Phosphorus crosslinks, in presence of a crosslinker, to form char
    - Nitrogen controls pH and has synergistic effect
  - **Questions**
    - Can we develop halogen-free FR chemistry containing P/N to provid

synergy? If so, how effective could it be for different fibers?

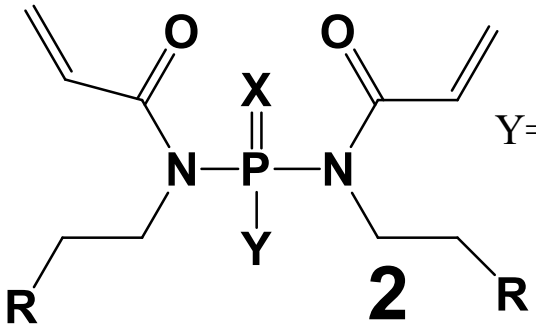
Why Do We Care About This Research?

- **Overall Objectives**
  - Develop a halogen-free flame retardant treatment for nonwoven polypropylene and polyester that is durable and self-extinguishing with no dripping or smoking during vertical flame testing
  - Treatment should achieve graft polymerization *via* plasma or UV treatment
- **Deliverables**
  - Halogen-free flame retardant monomers
  - Identify optimum FR monomer/crosslinker chemistry
  - Identify optimum UV exposure time to graft FR onto nonwoven polypropylene and polyester
  - Determine structure/property relationship of FR monomers (**1-6**)
- **Accomplished in this project**
  - 6 halogen-free monomers developed
  - Monomers **4** &**6** showed self-extinguishing properties when applied to PP &PET

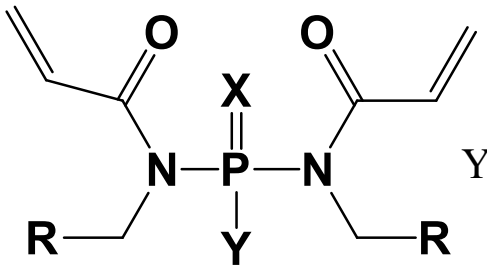
Structure-Property Relationships: Monomers 1-6



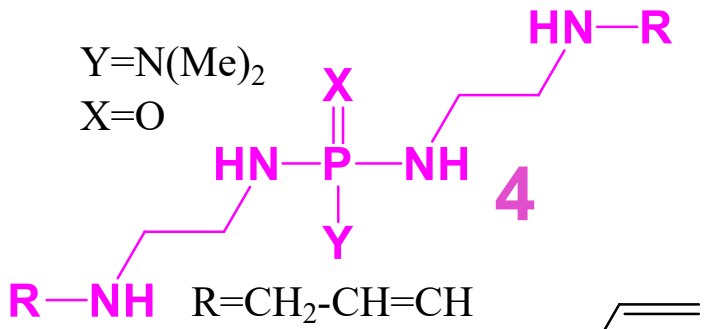
1 Y=OEt, X=O



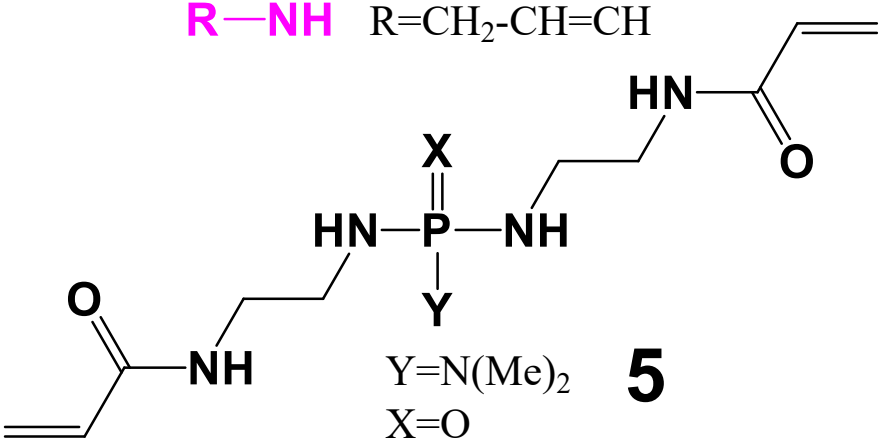
2 Y=N(Me)$_2$, X=O, R=CH$_2$OH



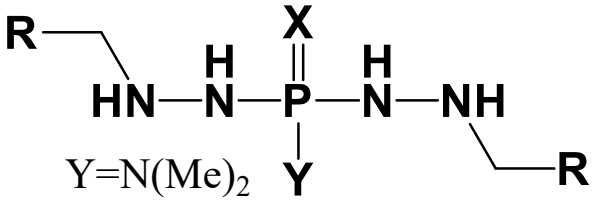
3 Y=N(Me)$_2$, R=CH$_2$OCO-CH=CH



4 Y=N(Me)$_2$, X=O, R=CH$_2$-CH=CH

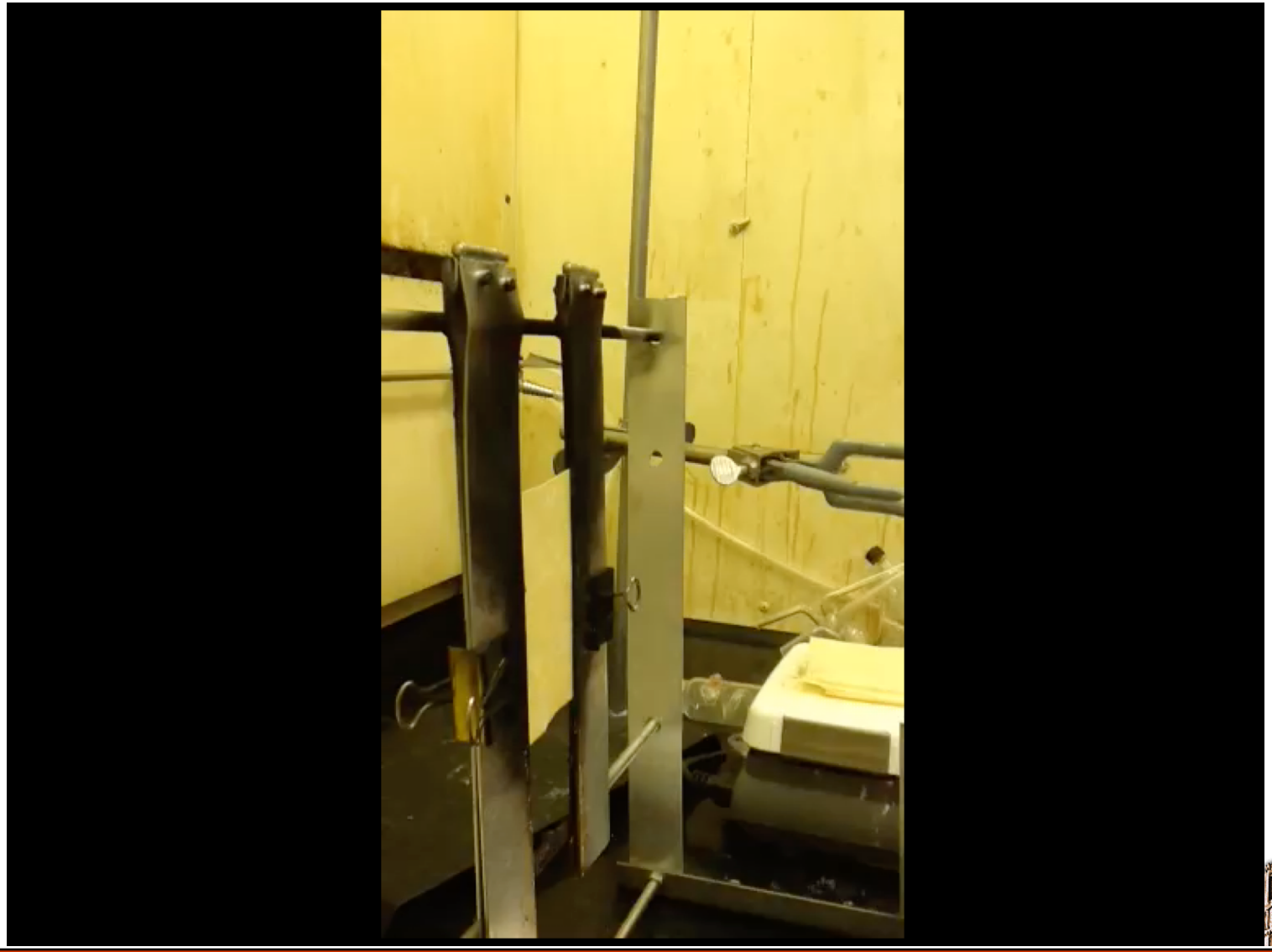


5 Y=N(Me)$_2$, X=O



6 Y=N(Me)$_2$, X=O, R=CH$_2$-CH=CH

Self-extinguishing properties on PET and PP



Conclusions

- Monomers 4 and 6 achieved the best self-extinguishing properties
- Developed chemistry Achieved
  - No melting or dripping
  - nontoxic smoke
- Good polymerization yield was achieved for all monomers
- Uniform char formation was achieved

El-Shafei's Research Group

Acknowledgements of Funding

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- Nike
- Eastman Chemicals
- USDA
- NTC
- NWI

THANK YOU

Questions