SOLAR FUELS
& NEXT GENERATION PHOTOVOLTAICS

UNC Energy Frontier Research Center

VISION

Provide the basic research to enable a revolution in collecting and converting sunlight into storable solar fuels.

MISSION

"We will combine the best features of academic and translational research to study light/matter interactions and chemical processes for the efficient collection, transfer, and conversion of solar energy into solar fuels and electricity."

ENERGY FRONTIER RESEARCH CENTER

The University of North Carolina at Chapel Hill

Duke UNIVERSITY | North Carolina Central University | NC STATE UNIVERSITY | RTI INTERNATIONAL | UF UNIVERSITY of FLORIDA

SOLAR FUELS & NEXT GENERATION PHOTOVOLTAICS

UNC Energy Frontier Research Center

MEETING GRAND CHALLENGE NEEDS

1. ***Controlling the basic architecture of matter*** *Both hard and soft, for catalysis, redox separation and electron and hole transport, and integration in devices for artificial photosynthesis*
2. ***Realizing the dream of nanoscience*** *by integrating functional molecular and nanoscale elements into micro- to macroscale devices*
3. ***Characterizing matter far from equilibrium*** *in excited states or as transiently stored redox equivalents and how to manipulate them for energy transduction on multiple length scales, from the molecular to the micron.*

MEETING BES BASIC RESEARCH NEEDS

Solar Water Splitting

BES Report 7, "Basic Research Needs for the Hydrogen Economy"
BES Report 8, "Basic Research Needs for Solar Energy Utilization."

Fundamental issues in electron transfer–driven catalysis in water oxidation and reduction and in CO_2 reduction to methanol and hydrocarbons.

BES Report 2, "Basic Research Needs in Catalysis for Energy Applications."

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THRUST AREAS

SOLAR FUELS

Solar Fuels: Catalysis and Materials

- *Light absorption & electron transfer driven catalysis in molecular assemblies and composite materials.*
- *Efficient devices for splitting water into H_2 and O_2, and reducing CO_2 to methanol and hydrocarbons.*

Next Generation Photovoltaics

- *Structurally controlled molecular assemblies & composites.*
- *Measurement & analysis of exciton dynamics & energy and charge transport.*
- *Design of new interfaces amenable to roll-to-roll nanostructure fabrication.*

Advanced Spectroscopy & Theory

- *Supporting Solar Fuels and Photovoltaics*
- *Cutting edge experimental methods & analysis of experimental data.*
- *National & international leader in theoretical studies & predicting and understanding scientific phenomena.*

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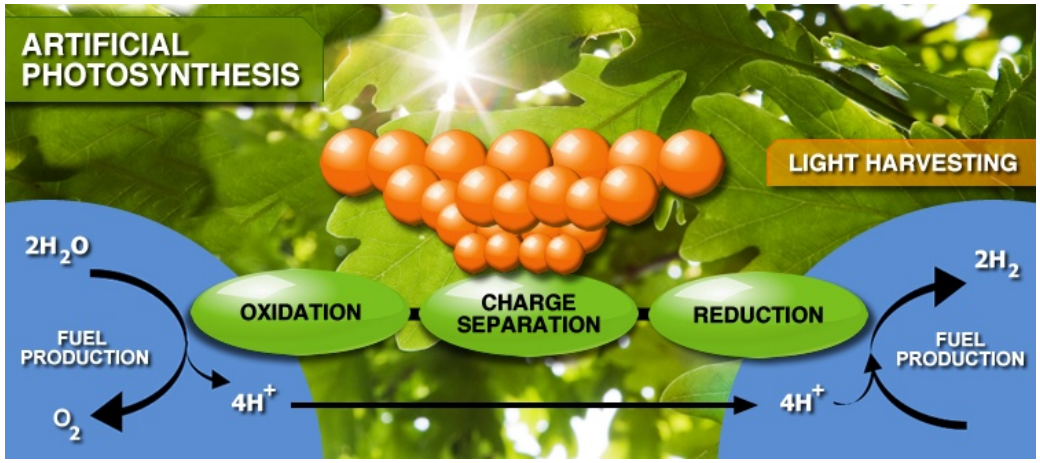
SOLAR FUELS



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People — *29 Faculty, 4 Scientific Staff, 12 Postdoctoral, 26 Graduate Students + Affiliates*

Collaborations — *Duke, NCSU, NCCU, U. Florida, RTI*

Partnerships — *Research Triangle Energy Consortium RTEC*
National Instruments

User Facilities — *Laser Laboratory, Fabrication Laboratory*

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ORGANIZATION CHART

SOLAR FUELS

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Advisory Boards
Internal & External

Industrial Partners
RTI, NI

EFRC Director
Meyer

Deputy Director
Papanikolas

Executive Assistant
Thauer

Assistant Director
Heyer

Executive Committee
Meyer, Papanikolas, Schauer, Pinschmidt
Baucom (Executive Consultant)

Operations Council
Meyer, Papanikolas, Schanze*, Lin

Senior Research Scientist
Spectroscopy - Brennaman

Senior Research Scientist
Catalysis - Concepcion

* **Collaborating Partner Site**

Solar Fuels Catalysis (Meyer)

SF Catalysis Water Oxidation (Meyer)

Faculty
Brookhart
Meyer
Murray
Templeton
Yousaf

Staff
Hoertz*

RA
Finniss, Jurss
Luo, Norris

SF Catalysis CO_2 Reduction (Brookhart)

Faculty
Brookhart
Meyer
Schauer

PostDoc
Ess, Lowry
Weinberg

RA
Kent

Solar Fuels Materials (Lin)

SF Materials Metal Oxides (Murray)

Faculty
Lin
Meyer
Murray
Qin
Wu

RA
Bjorge, deKrafft
Gambardella
Mogilevsky, Ren

SF Materials Framework Materials (Lin)

Faculty
Lin
Maggard*
Meyer

PostDoc
Lin*
Xie

RA
deKrafft
Kent

Advanced Spectroscopy& Theory (Papanikolas)

Solar Fuels Photophysics (Forbes)

Faculty
Forbes, Liu
McNeil, Meyer
Moran, Schauer,
Papanikolas
Whitten*, Yang*

PostDoc
Hu*, Knight, Papas*
Lebedeva,Tsuchiya*

RA
Brosnan, House
Miller
Westlake

Energy Transport/ CT Dynamics (Papanikolas)

Faculty
Beratan*, Fecko
Meyer
Papanikolas
Papoian, Therien*
Yang*

PostDoc
Knight
Kuznetsov*

RA
Bettis, Materese
McNeil, Rawson*

Photovoltaics & Devices (Schanze*)

Photovoltaics Assemblies (Schanze*)

Faculty
Ashby, Meyer
Papanikolas
Reynolds*
Schanze*, Taylor*
Therien*, Waters

PostDoc
Sun*

RA
Griffin*, Rawson*
Puodziukynaite*
Rochette, Wilger

Devices Patterned Electrodes (Samulski)

Faculty
DeSimone
Lopez
Samulski
You

Staff
Hoertz*

RA
Ghosh, Hampton
Ok, Stuart
Williams

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Artificial Photosynthesis – Solar Fuels

SOLAR FUELS

$2\ H_2O + 4\ h\nu \longrightarrow 2H_2 + O_2 \quad (\Delta G^o = 4.92\ eV,\ n = 4)$

$2\ H_2O \longrightarrow O_2 + 4\ H^+ + 4\ e^- \quad (E^o = -1.23\ V)$

$4\ H^+ + 4\ e^- \longrightarrow 2\ H_2 \quad (E^o = 0\ V)$

$2\ H_2O + CO_2 + 8\ h\nu \longrightarrow CH_4 + 2O_2 \quad (\Delta G^o = 10.3\ eV,\ n = 8)$

$2\ H_2O \longrightarrow O_2 + 4H^+ + 4e^- \quad (E^o = -1.23\ V)$

$CO_2 + 8H^+ + 8e^- \longrightarrow CH_4 + 2\ H_2O \quad (E^o = -0.22\ V)$

(900 nm = 1.38 eV)

- ***Load Leveling for electric power generation***
- ***Use existing energy infrastructure***

Water oxidation is a key half reaction

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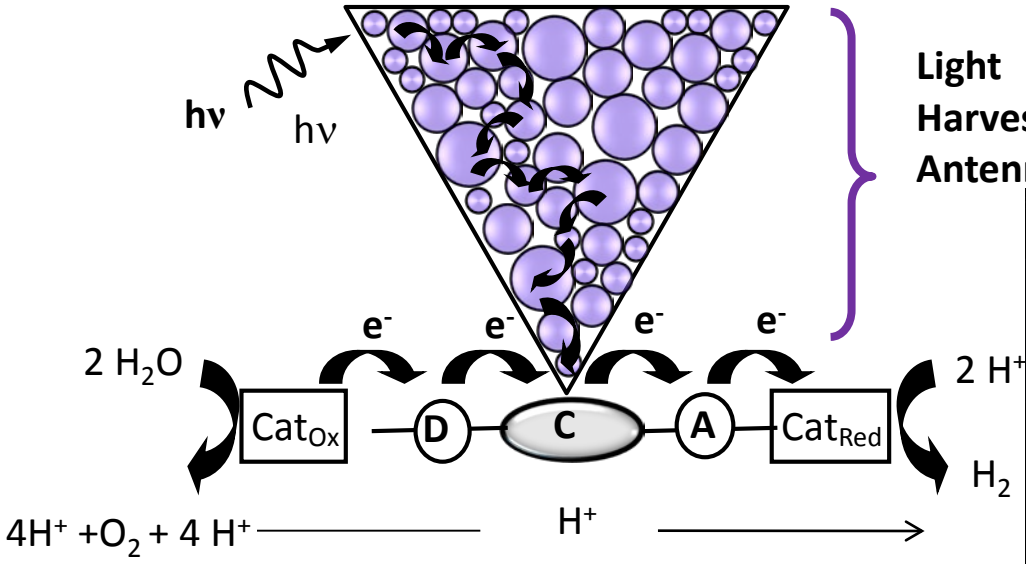
Modular Approach to Artificial Photosynthesis Molecular Assemblies

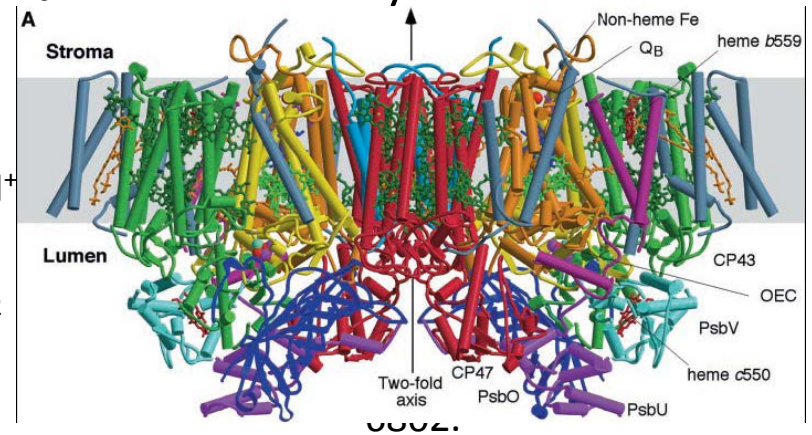
SOLAR FUELS

- **Light absorption**
- **Electron transfer quenching**
- **Vectorial electron/proton transfer, redox splitting**
- **Catalysis of water oxidation and reduction**



D = Electron Donor
C = Chromophore
A = Electron Acceptor

Photosystem II



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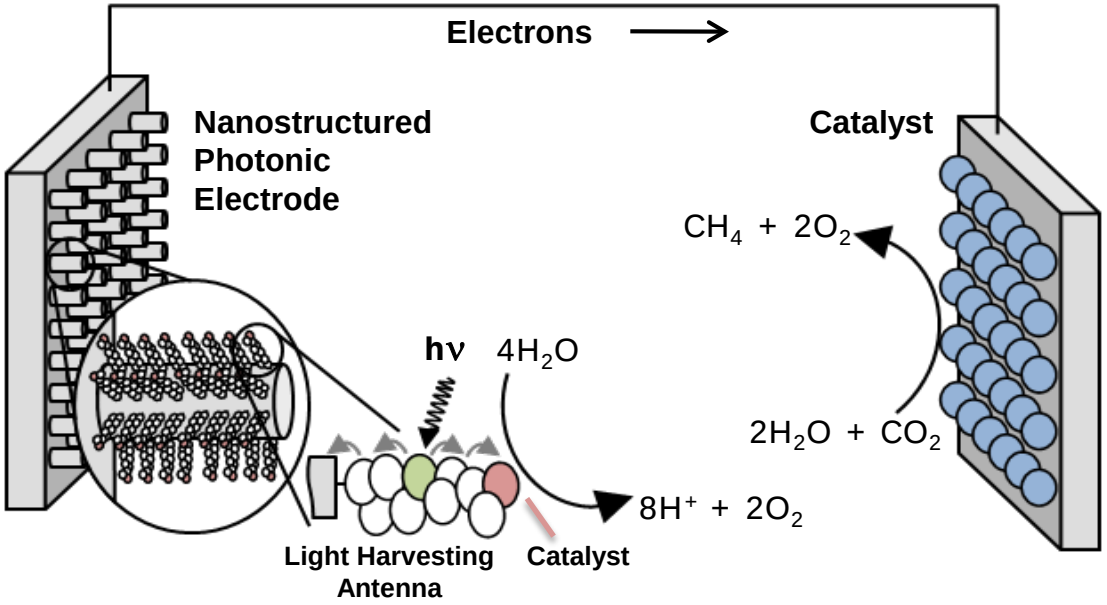
Dye Sensitized Photoelectrochemical Cells (DS-PEC) – A Modular Approach

SOLAR FUELS

- *Light absorption*
- *Electron transfer quenching by injection*
- *Inter-electrode e^-/H^+ activation of Cat_{red}*
  Intramolecular activation of Cat_{ox}
- *Catalysis of water oxidation and reduction*

Keep it simple!



Performance Limitations and Requirements

- *Visible-near IR light absorption (to 900 nm = 1.38 eV) with absorbance > 1*
- *Redox potentials, ($E^o(C^{+/0})$), $E^o(Cat_{red})$, sufficient for water oxidation or water (H^+)/CO_2 reduction*
- *Fast, efficient photoinjection, slow back electron transfer*
- *Rapid electron/proton activation of multi-electron catalysts*
- *Stable surface binding with electroactivity*
- *Rapid catalytic reactions; rate > 10 mA/cm²; turnover rate > 1 msec*
- *Robust catalytic behavior*
- *Scaleup*

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Structured OPV Assemblies

SOLAR FUELS

OPV

ADVANTAGES

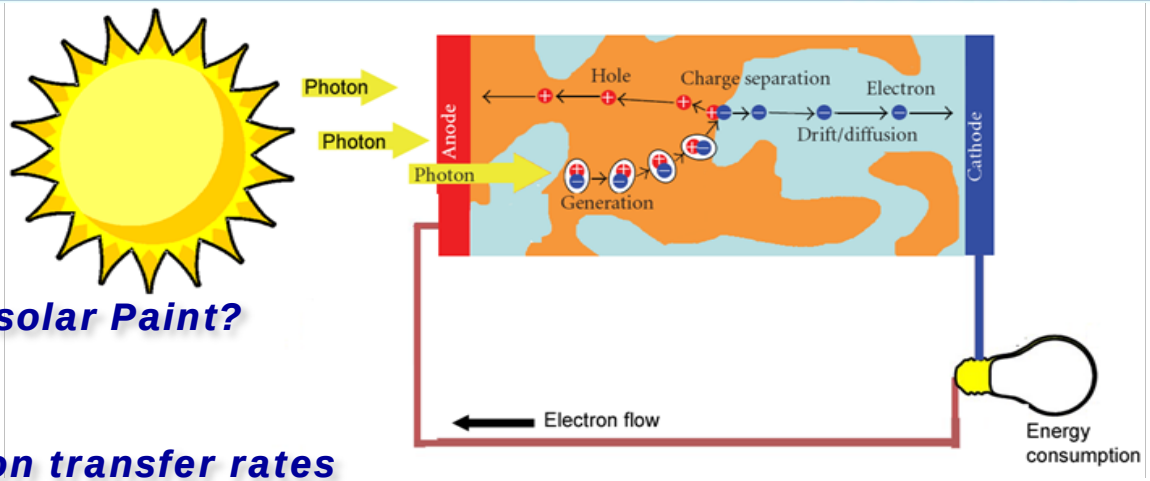
Inexpensive, abundant

Easily processed - Solar shingles, solar Paint?

DISADVANTAGES

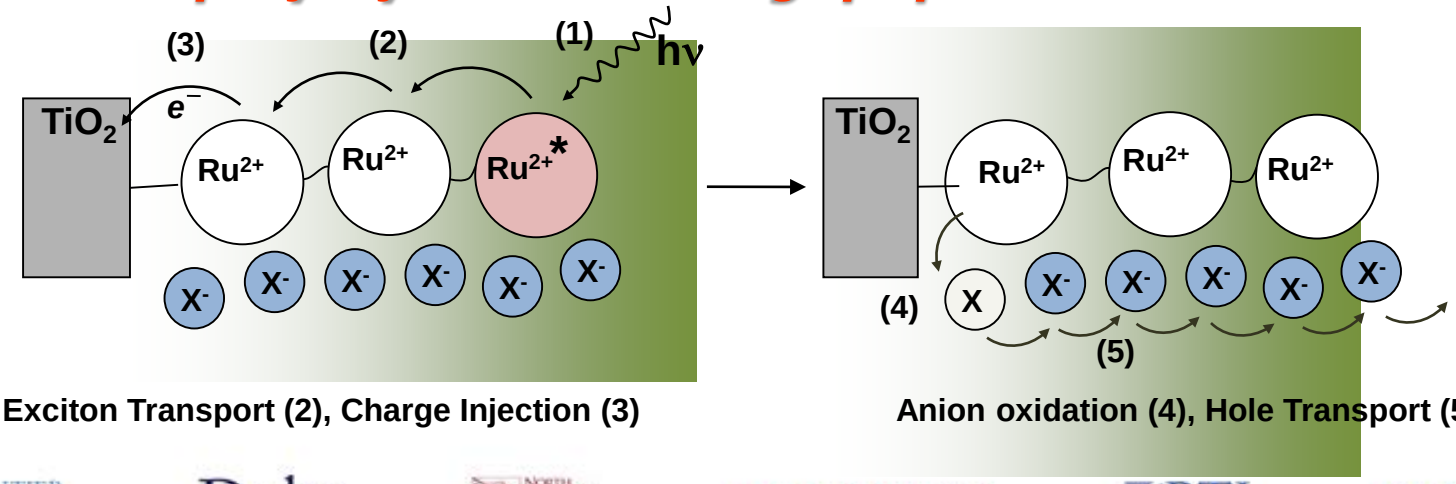
Bad physics - slow exciton/electron transfer rates

Competitive electron/hole transfer recombination



Bulk Heterojunction OPV

Structurally controlled long range electron/energy transport in polystyrene and oligopeptide assemblies



Excitation (1), Exciton Transport (2), Charge Injection (3)

Anion oxidation (4), Hole Transport (5)

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From Photons to Fuels

SOLAR FUELS

SCIENCE

Translational Research

DEVICES

Catalyst Design & Development

- Water Oxidation Catalysts
- CO_2 Reduction Catalysts

Component Design & Development

- Light-Harvesting Systems
- Metal Oxide Electrodes

Integration

- Light Harvesting/Catalyst Integration
- Surface Attachment

Devices

- Photoelectrochemical Cell Design & Development

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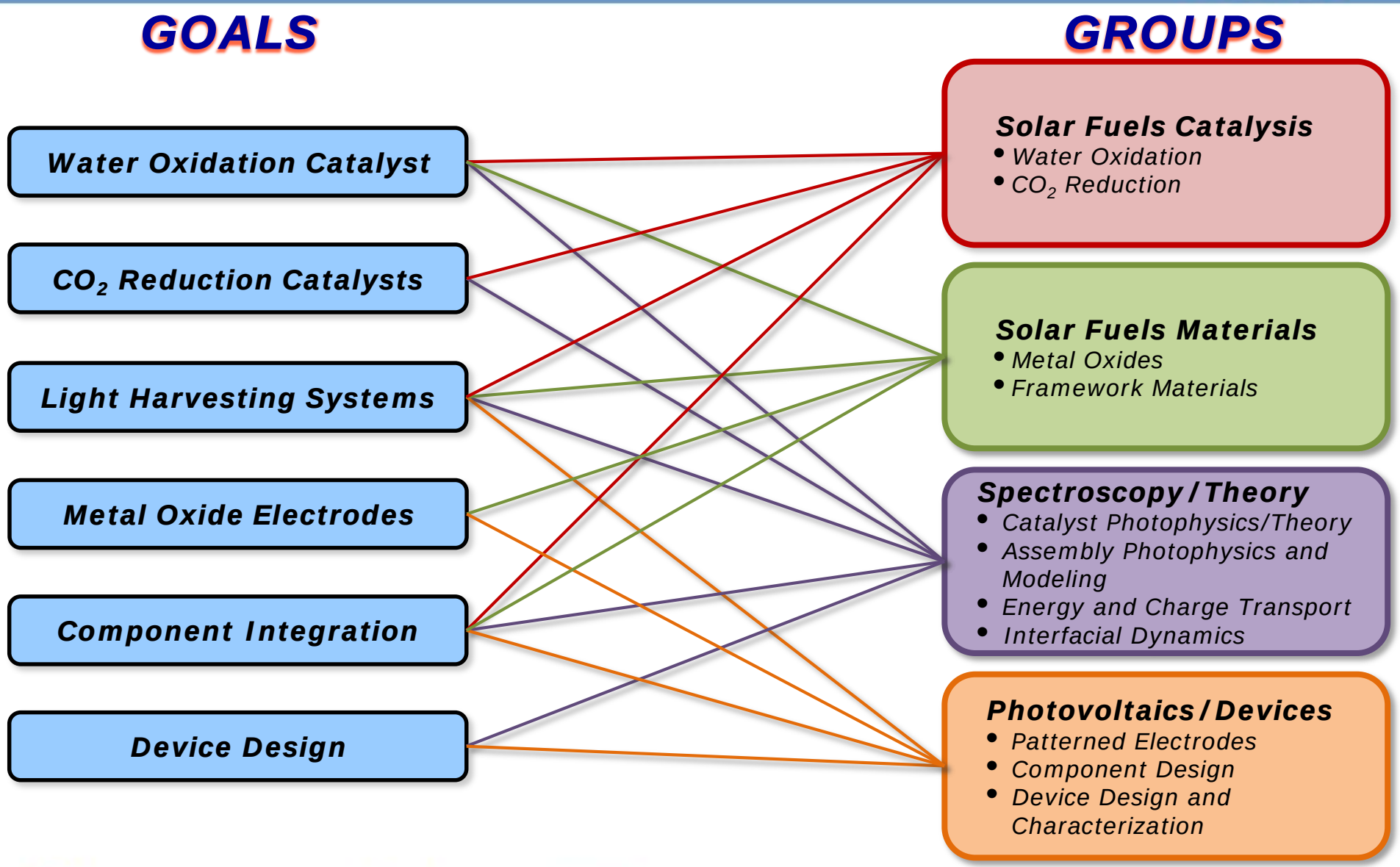
From Photons to Fuels
Synergy & Collaboration

SOLAR FUELS



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CONFERENCES & COMMUNICATIONS

SOLAR FUELS

- **Solar Energy Research Center National Scientific Conference**
  Solar Fuels and Energy Storage: The Unmet Needs
  ➡ **UNC EFRC Members - 4 presentations, 20 posters**

- **Planning First UNC EFRC Science Conference May 11-12, 2010**

- **4 Groups**
  - Solar Fuels Catalysis
  - Solar Fuels Materials
  - Advanced Spectroscopy & Theory
  - Photovoltaics & Devices

8 Teams – Biweekly meetings
Quarterly Center Meetings

Collaborative, Cross-cutting,
Inter-Institutional, Interdisciplinary

- **Visiting Scholar/Speaker Program**
  8 visiting speakers, 3 visiting scholars

- **Communications**
  Sharepoint Intranet Collaboration Portal
  Inter-Institutional Videoconferencing

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ACCOMPLISHMENTS

SOLAR FUELS

- **Public Outreach Forum**
  A Sustainable Energy Future – Mapping the Way
  - Assess the Magnitude of the Energy Problem
  - Evaluate the Capability of Current Technologies
  - Examine Prospects for Future Technologies
  - Explore the Transition to Our Energy Future
- **Laser Laboratory, Fabrication Laboratory**
- **Collaborations**
  RTEC, NI, others in process
- **Six UNC EFRC Publications**
- **Proposals**
  - DOE Energy Innovation Hub
    Fuels from Sunlight
  - DoD ONR Multidisciplinary University Research Initiative MURI Proposal
    Photoelectrochemical Reduction of Carbon Dioxide to Liquid Fuels
  - DOE SciDAC
    Enhancing Productivity of Materials Discovery Computations for Solar Fuels & Next Generation Photovoltaics
  - NSF Integrative Graduate Education & Research Traineeship IGERT Proposal
    Renewable Energy & Sustainability
  - Congressional Appropriation (UNC Priority) – EFRC Scientific Computing