

**Final Report DOE DE-SC0015750**

**Institution: Yale University**

**Title: 2016 TSRC Summer School on Fundamental Science for Alternative Energy**

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**Report Date: 8/25/17**

**Period of Report: 6/15/16-6/14/17**

The 2016 TSRC Summer School on Fundamental Science for Alternative Energy introduced principles, methods, and approaches relevant to the design of molecular transformations, energy transduction, and current applications for alternative energy. Energy and environment are likely to be key themes that will dominate the way science and engineering develop over the next few decades. Only an interdisciplinary approach with a team-taught structure as presented at the 2016 TSRC Summer School can be expected to succeed in the face of problems of such difficulty. The course inspired a new generation of 24 graduate students and 2 post-docs to continue work in the field, or at least to have something of an insider's point of view as the field develops in the next few decades.

The list of topics and instructors, in order of appearance, included: Gary Brudvig (GB) who introduced the scientific basis behind environmental changes, the problem that drives the whole alternative energy project, and provided fundamental concepts on design of bioinspired photocatalytic assemblies, including biophysical principles of light-harvesting, charge separation and fuel production revealed by studies of the natural systems and related to artificial electrochemical processes. Ana Moore (AM) discussed approaches for synthesis of artificial antenna molecular frameworks, solar light harvesting and characterization of energy/charge transfer in synthetic molecular assemblies. Elena Galoppini (EG) introduced designs and studies of rigid molecular linkers for the functionalization of semiconductor nanoparticles with dyes, chromophores and redox active groups, including nanoparticle-linker-donor systems for fundamental studies of nanoparticle electronic interactions as well as practical applications for photovoltaics (solar cells), sensors and other devices. Charles Schmittenmaer (CS) discussed properties of semiconductor materials that make up photocatalytic solar cells and characterization based on spectroscopic methods. Eric Bittner (EB) introduced theoretical aspects of charge transport in organic electronics, including molecular modeling methods for simulations of electronic excitations relevant to organic photovoltaic devices. Victor Batista (VB) introduced computational methods for design and characterization of molecular systems and applications to solar cells, photocatalysis and biomimetic water-splitting.

## FACULTY

**Gary Brudvig** (GB) (natural photosynthesis and biomimetic systems, electrochemistry)

**Ana Moore** (AM) (antenna synthesis, characterization of energy/charge transfer)

**Elena Galoppini** (EG) (design of rigid linkers, dye-nanoparticle electronic interactions)

**Charlie Schmittenmaer** (CS) (semiconductor materials, spectroscopy of carriers)

**Eric Bittner** (EB) (charge transport in organic electronics, organic photovoltaics)

**Victor Batista** (VB) (theory and computational modeling PSII, DSSC, photocatalysis)

## Meeting Schedule

	<b>Tuesday June 21</b>	<b>Wednesday June 22</b>	<b>Thursday June 23</b>
<b>Morning</b>	<b>Research Interests</b>	<b>Significance + Fundamentals</b>	<b>Transport+ Semiconductors</b>
<b>9:00-9:30</b>	<i>G. Brudvig</i>	<i>G. Brudvig:</i>	<i>Schmittenmaer:</i>
<b>9:30-10</b>	<i>A. Moore</i>	Lecture 1	Lecture 1
<b>10-10:30</b>	E. Bittner	Discussion 1	Discussion 1
<b>Break</b>			
<b>11-11:30</b>	<i>E. Galoppini</i>	<i>A. Moore:</i>	<i>E. Bittner:</i>
<b>11:30-12</b>	<i>Schmittenmaer</i>	Lecture 1	Lecture 1
<b>12-12:30</b>	<i>V. Batista</i>	Discussion 1	Discussion 1
<b>Afternoon</b>	<b>Research Interests</b>	<b>Natural/Artificial Light Harvesting</b>	<b>Molec/Electronic Dynamics</b>
<b>2:00-2:30</b>			
<b>2:30-3:00</b>			
<b>3-3:30</b>			
<b>Break</b>			
<b>4-4:30</b>	Student G1	<i>E. Galoppini:</i>	<i>V. Batista</i>
<b>4:30-5</b>	Student G2	Lecture 1	Lecture 1
<b>5-5:30</b>	Student G3	Discussion 1	Discussion 1
<b>Evening</b>			
<b>6:00-8:00</b>			Bear Creek Cookout

	Friday June 24	Saturday June 25
<b>Morning</b>	<b>Significance + Fundamentals</b>	<b>Transport+ Semiconductors</b>
<b>9:00-9:30</b>	<i>A. Moore:</i>	<i>Schmuttenmaer:</i>
<b>9:30-10</b>	Lecture 2	Lecture 2
<b>10-10:30</b>	Discussion 2	Discussion 2
<b>Break</b>		
<b>11-11:30</b>	<i>G. Brudvig:</i>	<i>V. Batista:</i>
<b>11:30-12</b>	Lecture 2	Lecture 2
<b>12-12:30</b>	Discussion 2	Discussion 2
<b>Afternoon</b>	<b>Natural/Artificial Light Harvesting</b>	<b>Molec/Electronic Dynamics</b>
<b>2:00-2:30</b>		
<b>2:30-3:00</b>		
<b>3-3:30</b>		
<b>Break</b>		
<b>4-4:30</b>	<i>E. Bittner:</i>	<i>Students:</i>
<b>4:30-5</b>	Lecture 2	Discussion
<b>5-5:30</b>	Discussion 2	
<b>Evening</b>		
<b>6:00-8:00</b>		