

## NARRATIVE

The 2019 TSRC Center Summer School on Fundamental Science for Alternative Energy Summer School will introduce 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 can be expected to succeed in the face of problems of such difficulty hence the team-taught structure of the TSRC Summer School. We hope this course will inspire a new generation of scientists to continue work in the field, or at least to have an insider's point of view as the field develops.

The list of topics, all DOE-relevant, and instructors includes: **Gary Brudvig** will introduce the scientific basis behind climate change and will provide 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** will discuss approaches for synthesis of antenna molecular frameworks, solar light harvesting and characterization of energy/charge transfer in synthetic molecular assemblies based on proton-coupled electron transfer (PCET) mechanisms. **Thomas Moore** will introduce a discussion on the global carbon cycle, global scale photosynthesis, human appropriation of net primary production and issues related to sustainability leading into the myriad forms of artificial photosynthesis including recent work on reengineered photosynthesis, with emphasis on efficiency of converting solar energy to electrical or chemical potential energy. **Charles Schmuttenmaer** will discuss properties of semiconductor materials that make up photocatalytic solar cells and characterization based on spectroscopic methods. **Eric Bittner** will introduce theoretical aspects of charge transport in organic electronics, including molecular modeling methods for simulations of electronic excitations relevant to photovoltaics. **Victor Batista** will introduce computational methods for design and characterization of molecular systems and applications to solar cells, photocatalysis and biomimetic water splitting.

TSRC provides equipped meeting and poster rooms, accommodations, dining facilities, audiovisual support and a staffed office. The Summer School site is accessible for people with disabilities and when registering for the conference such people will be able to identify any special needs so that the conference organizers can accommodate those needs.

**Summer School Location, Expected Number of Attendants, and Leaders.** The first Telluride School on Fundamental Science of Alternative Energy (Summer School) was in 2014 and led by Victor Batista and Gary Brudvig of Yale University and followed by a 2016 school. In 2016, the Summer School had 6 faculty members (Ana Moore of Arizona State University, Elena Galoppini of Rutgers University, Charles Schmittenmaer of Yale University, and Eric Bittner of University of Houston as well as the founders) teaching 26 graduate students and 3 postdoctoral associates. The goal of the 2019 Summer School is to bring in around 26 graduate student and postdoctoral associate attendees, and this proposal requests the funds to help us achieve this goal.

The 2019 line-up of faculty have extensive experience in running similar workshops and in holding other relevant leadership positions:

Gary Brudvig (Yale University):

1. Co-founder and faculty for the Summer School in 2014, 2016.
2. Associate Editor of *Biochemistry*.
3. Current Director of the Energy Sciences Institute at Yale University.
4. Chair of the Chemistry Department at Yale University.

Victor Batista (Yale University):

1. Co-founder and faculty for the Summer School in 2014, 2016.
2. Chair of the 2019 Gordon Research Conference Vibrational Spectroscopy.
3. Vice-chair of the 2014 Gordon Research Conference Vibrational Spectroscopy.
4. Co-organizer of the 2019 KI-Net Conference on Mathematical and Computational Methods in Quantum Chemistry at Yale University.
5. Co-organizer of the 2013 Summer School on Mathematical and Computational Methods in Quantum Dynamics at the University of Wisconsin-Madison.
6. Co-organizer of the 2013 Banff workshop on Mathematical Methods in Quantum Molecular Dynamics, Alberta, Canada.
7. Co-organizer of the 2010 Symposium on Quantum-Classical Modeling of Chemical Phenomena at the University of Maryland, College Park.
8. Co-organizer and chair of the 2010 ACS Symposium on Renewable Energy; and organizer of the 2008 Cokerfest Symposium on Quantum Dynamics at Boston University.
9. Senior Editor of the *Journal of Physical Chemistry C*.

Charles Schmittenmaer (Yale University):

1. Faculty for the Summer School in 2014, 2016.
2. Co-organizer for the DOE-NIH-NSF Workshop on Opportunities in THz Science in 2004.
3. Co-organizer for the THz Workshop held at the SPIE annual meeting in Denver in 2004.
4. Director of Graduate Studies at Yale University.

Eric Bittner (University of Houston):

1. Co-organizer of the 2nd PRC workshop on "Energy Flow Dynamics in Biomaterial Systems" in Paris in 2007.
2. Member of the American Physical Society Committee on Careers and Professional Development.
3. Guest Editor for the Journal of Physical Chemistry B (Festschrift honoring Robert E. Wyatt).

4. Faculty for the Summer School in 2016.

Ana Moore (Arizona State University):

1. Faculty for the Summer School in 2014, 2016.
2. Previous Assistant Chair for Graduate Studies.
3. Member of the Organizing Committee. 21st Interamerican Photochemical Society, Mendoza Argentina in 2011.
4. Subtask Leader for the Center for Bio-Inspired Solar Fuel Production.

Thomas Moore (Arizona State University):

1. 2011- Distinguished Sustainability Scientist
2. 2011- Regents' Professor Global Institute of Sustainability
3. 2014, 2016- Faculty for the TSRC Summer School in Alternative Energy

### **TSRC Summer School Plan.**

The first session (Saturday morning) will focus on introducing the research interests and topics of expertise of the faculty teaching for the Summer School.

The second session (Saturday afternoon) will focus on discussing the research interests and current research work by the graduate students and postdocs at their corresponding institutions. Please, bring a 5 minute presentation of your research interests.

The third session (Sunday morning) will focus on the significance and fundamentals of alternative energy science, as taught by Gary Brudvig and Ana Moore. There will be both lecture portions and discussion portions with the audience.

The fourth session (Sunday evening) will focus on the global carbon cycle, global scale photosynthesis, human appropriation of net primary production by Thomas Moore. There will be both a lecture portion and a discussion portion with the audience.

The fifth session (Monday morning) will focus on transport and semiconductors, as taught by Charles Schmittenmaer and Eric Bittner. There will be both lecture portions and discussion portions with the audience.

The sixth session (Monday evening) will focus on molecular and electronic dynamics, as taught by Victor Batista. There will be both a lecture portion and a discussion portion with the audience.

The seventh session (Tuesday morning) will continue on the topic of the significance and fundamentals of alternative energy science, as taught by Gary Brudvig and Ana Moore. There will be both lecture portions and discussion portions with the audience.

The eighth session (Tuesday evening) will continue on the topic of natural and artificial light harvesting, as taught by Eric Bittner. There will be both a lecture portion and a discussion portion with the audience.

The ninth session (Wednesday morning) will continue on the topic of transport and semiconductors, as taught by Charles Schmuttenmaer and Victor Batista. There will be both lecture portions and discussion portions with the audience.

The tenth and final session (Wednesday evening) by Thomas Moore will focus on sustainability leading into the myriad forms of artificial photosynthesis, including recent work on reengineered photosynthesis, with emphasis on efficiency of converting solar energy to electrical or chemical potential energy. There will be both a lecture portion and a discussion portion with the audience.

In closing, the speakers are leaders in the field of alternative energy, and many of them have been speakers at the previous Summer School. Among the 6 speakers, 2 are women, who serve as important role models for many female students and postdoctoral

fellows. The idea here is to develop this Summer School as a "training ground" for scientists in alternative energy, broadly defined. The participants are all graduate students and postdoctoral associates at the beginning of their careers. The continued participation of these young researchers in this Summer School demonstrates their commitment to this field, and the growing importance of it in the alternative energy community. Overall, we firmly believe that by supporting the 2019 Summer School, the pipeline of domestically trained graduate students and postdocs in the exciting area of alternative energy, the major challenge facing not only scientists, but all of humanity, in the 21<sup>st</sup> century, will be strengthened.

### **Funds Requested**

The goal of this request is to support exceptional graduate students and postdoctoral researchers from diverse backgrounds to attend the 2019 Summer School. Our total request for support from DOE is \$10,000.

### **Methods of Announcement**

The methods of announcement to the community for this Summer School include emails through the TSRC and through mailing lists of EFRC's, emails to PI's involved in solar energy research, and announcements at conferences. The Workshop Details are given on the TSRC website.

### **Costs**

All conferees are expected to attend the entire meeting. The registration fee at the TSRC is expected to be approximately \$390 per attendee.

## PROGRAM

Friday June 14	Saturday June 15	Sunday June 16	Monday June 17
<b>Morning</b>	<b>Research Interests</b>	<b>Natural Photosynthesis</b>	<b>Transport+ Semiconductors</b>
<b>9:00-9:30</b>	G. Brudvig	G. Brudvig:	Schmittenmaer:
<b>9:30-10:00</b>	A. Moore	Lecture 1	Lecture 1
<b>10:00-10:30</b>	E. Bittner	Discussion 1	Discussion 1
<b>Break</b>			
<b>11-11:30</b>	T. Moore	A. Moore:	E. Bittner:
<b>11:30-12</b>	Schmittenmaer	Lecture 1	Lecture 1
<b>12-12:30</b>	V. Batista	Discussion 1	Discussion 1
<b>Lunch Break</b>		<b>Bear Creek Hike/Lunch</b>	
<b>Afternoon</b>	<b>Research Interests</b>	<b>Group Hike</b>	<b>Team work</b>
<b>2:00-4:00</b>	Student G1		<b>5 Groups work on text for slides</b>
<b>Break</b>			
<b>4:30-6:00</b>	Badges	<b>Carbon Cycle</b>	
	Student G2	T. Moore	V. Batista
		Lecture 1	Lecture 1
		Discussion 1	Discussion 1
<b>Evening</b>			
<b>6:00-8:00</b>			Restaurant

	<b>Tuesday June 18</b>	<b>Wednesday June 19</b>
<b>Fundamentals + Morning</b>	<b>Fundamentals</b>	<b>Transport+ Semiconductors</b>
<b>9:00-9:30</b>	<i>A. Moore:</i>	<i>Schmittenmaer:</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>Lunch Break</b>		
<b>Afternoon</b>		
<b>2:00-2:30</b>	<b>Free</b>	<b>6 groups work</b>
<b>2:30-3:00</b>	<b>(Telluride Brewing Co.)</b>	<b>on text for slides</b>
<b>3-3:30</b>		
<b>Break</b>		
<b>4-4:30</b>	<i>E. Bittner:</i>	<b>Sustainability</b> <i>T. Moore:</i>
<b>4:30-5</b>	Lecture 2	Lecture 2
<b>5-5:30</b>	Discussion 2	Discussion 2
<b>Evening</b>	Town Talk	Picnic all-TSRC
<b>6:00-8:00</b>		