

# Research Opportunities in Photochemistry, Solar Energy & Advanced X-ray Methods

June 16-17, 2016  
SLAC National Accelerator Laboratory  
Menlo Park, CA

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## Agenda

### Thurs. June 16 - Plenary (Bldg. 53 Panofsky Auditorium)

8:00 AM	<i>breakfast</i>	
8:30 AM	Welcome	<i>K. Gaffney-SSRL M. Dunne-LCLS</i>
8:45 AM	Robust Catalysts for Solar-Driven Water Splitting	<i>Harry Gray Cal Tech</i>
9:15 AM	<i>discussion</i>	
9:30 AM	Semiconductor Nanocrystals and Solar Energy Conversion: Challenges and Opportunities	<i>Victor Klimov LANL</i>
10:00 AM	<i>discussion</i>	
10:15 AM	<i>break</i>	
10:35 AM	Element-, site- and orbital-specific probes of chemical interactions – So what?	<i>Philippe Wernet BESSY</i>
11:05 AM	<i>discussion</i>	
11:20 AM	Chemical Dynamics in an X-ray Scattering Perspective	<i>Martin Nielsen T.U. Denmark</i>
11:50 AM	<i>discussion</i>	
12:05 PM	<i>lunch</i> (Bldg. 48 Redwood Lobby/Breezeway)	

### *Breakout: Nano- and solid state materials for solar energy conversion* (Bldg. 48 Redwood Rooms C/D) *Leads: Aaron Lindenberg, Diling Zhu, Aymeric Robert*

1:20 PM	<i>Introduction</i>	<i>Aaron Lindenberg SLAC</i>
1:25 PM	X-ray spectroscopy at SLAC: Capabilities, science program and future directions	<i>Dimosthenis Sokaras SLAC</i>
1:40 PM	<i>discussion</i>	

1:50 PM	Using Near-Edge Absorption and Decay of Core-Excited States to Probe Charge and Exciton Transfer in Organic Semiconductor Assemblies	Alex Ayzner UCSC
2:15 PM	<i>discussion</i>	
2:30 PM	Time-domain ab initio studies of excited state dynamics in solar energy materials	Oleg Prezhdo USC
2:55 PM	<i>discussion</i>	
3:10 PM	<i>break</i>	
3:25 PM	Resolving reversible optically-driven phase transitions in hybrid perovskites	Naomi Ginsberg U.C. Berkeley
3:50 PM	<i>discussion</i>	
4:05 PM	Chemical approaches to addressing the instability and toxicity of lead-halide perovskite absorbers	Hemamala Karunadasa Stanford
4:30 PM	<i>discussion</i>	
4:45 PM	<i>discussion and contributed talks</i>	
6:00 PM	<i>dinner - on your own</i>	

**Breakout: Molecular materials for solar energy conversion  
(Bldg. 48 Redwood Rooms A/B)**

**Leads: Amy Cordones-Hahn, Bill Schlotter, Dennis Nordlund**

1:20 PM	Excited State Processes in Pt(II) Charge Transfer Dimers	Phil Castellano N.C. State
1:45 PM	<i>discussion</i>	
2:00 PM	X-ray Methodology: SSRL	Dennis Nordlund SLAC
2:20 PM	<i>discussion</i>	
2:40 PM	<i>break</i>	
2:55 PM	1st invited speaker: short talk	Alex Ayzner
	<i>discussion</i>	
3:20 PM	2nd invited speaker: short talk	Shu Hu
	<i>discussion</i>	
3:45 PM	3rd invited speaker: short talk	Kasper Kjaer
	<i>discussion</i>	
4:10 PM	breakout contributed talks and discussion	TBD
5:30 PM	<i>break</i>	
6:00 PM	<i>dinner - on your own</i>	

**Breakout: Fundamental chemistry and physics of light driven phenomena in molecular and nanomaterials (Bldg. 53 Panofsky Auditorium)**

*Leads:*

**Mike Minitti, Thomas Wolf, Josh Turner**

1:20 PM	Using Femtosecond X-rays to Probe Ultrafast Photochemistry in Solution	<i>Munira Khalil U. Washington</i>
1:45 PM	<i>discussion</i>	
2:00 PM	Vibronic Coherence as a Mechanistic Probe for Ultrafast Excited-state Dynamics in Transition Metal Complexes (invited)	<i>James McCusker Michigan State</i>
2:25 PM	<i>discussion</i>	
2:40 PM	Tabletop femtosecond XANES of transition metal complexes: does high-harmonic generation complement or compete with FELs?	<i>Josh Vura-Weis U. Illinois</i>
3:05 PM	<i>discussion</i>	
3:20 PM	<i>break</i>	
3:40 PM	Challenges in catalytic surface dynamics	<i>Jerry LaRue Chapman U.</i>
5:30 PM	<i>break</i>	
6:00 PM	<i>dinner - on your own</i>	

**Fri. June 17 - Plenary (Bldg. 51 Kavli Auditorium)**

8:30 AM	<i>breakfast</i>	
9:00 AM	Functional materials and interfaces for artificial photosynthesis	<i>Ian Sharp JCAP - LBNL</i>
9:30 AM	<i>discussion</i>	
9:45 AM	Ultrafast Dynamics in Molecular Assemblies for Solar Energy Conversion	<i>John Papanikolas U. North Carolina</i>
10:15 AM	<i>discussion</i>	
10:30 AM	<i>break</i>	
10:50 AM	Imaging Ultrafast Excited State Pathways in Transition Metal Complexes by X-ray Transient Absorption and Scattering Using X-ray Free Electron Laser Source	<i>Lin Chen Northwestern, ANL</i>
11:20 AM	<i>discussion</i>	
11:35 AM	Ultrafast charge separation at semiconductor/metal nanorod heterojunctions	<i>Tim Lian Emory U.</i>
12:05 PM	<i>discussion</i>	
12:20 PM	<i>Lunch</i>	

*(Bldg. 48 Redwood Lobby/Breezeway)*

**Breakout: Nano- and solid state materials for solar energy conversion  
(Bldg. 48 Redwood Rooms C/D)**

**Leads: Aaron Lindenberg, Diling Zhu, Aymeric Robert**

1:35 PM	<i>Introduction</i>	<i>Aymeric Robert SLAC</i>
1:40 PM	Exploring Nanoscale Thermal Transport via Time-Domain X-ray Scattering	<i>Mike Kozina SLAC</i>
1:55 PM	<i>discussion</i>	
2:05 PM	Using coherent x-rays to characterize phonon and thermal transport for energy applications	<i>Keith Nelson MIT</i>
2:30 PM	<i>discussion</i>	
2:45 PM	Atomic layer deposited metal oxides for efficient photoelectrochemical and photovoltaic transformations	<i>Paul McIntyre Stanford</i>
3:10 PM	<i>discussion</i>	
3:25 PM	breakout contributed talks, discussion and closeout prep	<i>TBD</i>
4:15 PM	<i>break</i>	

**Plenary Closeout**

4:30 PM	Breakout A presentation	
4:45 PM	<i>discussion</i>	
4:50 PM	Breakout B presentation	
5:05 PM	<i>discussion</i>	
5:10 PM	Breakout C presentation	
5:25 PM	<i>discussion</i>	
5:30 PM	<i>closing remarks</i>	

**Breakout: Molecular materials for solar energy conversion  
(Bldg. 48 Redwood Rooms A/B)**

**Leads: Amy Cordones-Hahn, Bill Schlotter, Dennis Nordlund**

1:35 PM	Light driven carbon dioxide reduction by water - dynamic X-ray spectroscopy as an essential tool	<i>Heinz Frei LBNL</i>
2:00 PM	<i>discussion</i>	
2:15 PM	X-ray Methodology: LCLS	<i>Bill Schlotter LCLS</i>
2:35 PM	<i>discussion</i>	
2:55 PM	1st invited speaker: short talk	<i>Junko Yano</i>
	<i>discussion</i>	
3:20 PM	2nd invited speaker: short talk	<i>Claudia Turro (tentative)</i>
	<i>discussion</i>	

3:45 PM breakout contributed talks and discussion *TBD*  
4:15 PM *break*

***Plenary Closeout***

4:30 PM Breakout A presentation  
4:45 PM *discussion*  
4:50 PM Breakout B presentation  
5:05 PM *discussion*  
5:10 PM Breakout C presentation  
5:25 PM *discussion*  
5:30 PM *closing remarks*

***Breakout: Fundamental chemistry and physics of light driven phenomena in molecular and nanomaterials (Bldg. 51 Kavli Auditorium)***

***Leads: Mike Minitti, Thomas Wolf, Josh Turner***

1:35 PM Ultrafast X-ray Studies of Interfacial Charge Transfer Dynamics *Oliver Gessner LBNL*  
2:00 PM *discussion*  
2:15 PM Instrument overview *Mike Minitti LCLS*  
2:40 PM breakout contributed talks, discussion & closeout prep  
4:15 PM *break*

***Plenary Closeout***

4:30 PM Breakout A presentation *TBD*  
4:45 PM *discussion*  
4:50 PM Breakout B presentation *TBD*  
5:05 PM *discussion*  
5:10 PM Breakout C presentation *TBD*  
5:25 PM *discussion*