

BIO-INSPIRED SOLAR ENERGY

Aims to improve our ability to use solar energy by learning lessons from the remarkable effectiveness of photosynthesis in plants, algae and photosynthetic bacteria.

This year, the program generated new insights into the role of the local environment (specifically local vibrations) on energy transfer in natural photosynthetic pigments in plants and algae, which have improved understanding of how organisms harness and use energy from the sun. Program chemists and materials scientists are also developing new catalysts and light-absorbing systems and applying the same spectroscopic methods to understand how these artificial systems mimic their natural counterparts. The aim is to determine new ways of maximizing their efficiency. The program is also exploring the potential for machine learning to accelerate materials discovery.

A number of meetings and workshops were held this year. The first program meeting, held in Montreal in October 2016, involved a full day of trainee and student presentations on collaborative research projects. This meeting was attended by new program members **Catherine Drennan** (Massachusetts Institute of Technology) and **Sharon Hammes-Schiffer** (University of Illinois at Urbana-Champaign), and new Advisory Committee member **Fraser Armstrong** (University of Oxford).

At the second program meeting, held in March 2017 in Cambridge, members met for two days to brainstorm and discuss the program's long-term goals. The focus was on understanding the synthetic biology and biophysical principles behind natural photosynthesis to design novel artificial systems with high efficiencies, as well as bottom-up approaches to solar energy conversion using bio-hybrid systems for light harvesting and energy storage.

To expand further on the program's materials development side, a May 2017 workshop in Cambridge, in collaboration with CIFAR's program in Learning in Machines & Brains, discussed new applications of machine learning for materials discovery.

Program Co-Director **Yoshua Bengio** (Université de Montréal) and program members exchanged ideas with machine learning experts from industry and government organizations, such as IBM, Toyota, TOTAL SA, Citrine Materials Informatics and AFOSR, on how artificial intelligence could accelerate the discovery of new catalysts and light-absorbing systems for solar energy conversion. Future work will explore the intersection between these fields, with the goal of enabling long-term energy solutions.

RESEARCH HIGHLIGHTS

Coherence (i.e., the communication or interaction between different electronic or vibrational states in a system) is a critical factor in solar energy transfer in biological systems. The key to creating high-efficiency artificial systems that can match or exceed the performance of natural systems is understanding how pigment molecules in plants and photosynthetic algae use coherence — specifically vibrational coherence and coupling to the local environment around the pigments — to facilitate energy transfer and flow. Fellows **Gregory Scholes** (Princeton University), **Alàn Aspuru-Guzik** (Harvard University), **Rienk van Grondelle** (Vrije Universiteit Amsterdam) and **Ted Sargent** (University of Toronto) published articles describing the latest advances in research related to light absorption, coherence and energy transfer in biological systems.

- Mirkovic T et al. 2017. Light absorption and energy transfer in the antenna complexes of photosynthetic organisms. *Chem Rev.* 117: 249-293.
- **Scholes G** et al. 2017. Using coherence to enhance function in chemical and biophysical systems. *Nature.* 543: 647-656.
- Brédas J-L et al. 2017. Photovoltaic concepts inspired by coherence effects in photosynthetic systems. *Nat Mater.* 16: 35-44.
- Blau SM et al. 2017. Local protein solvation drives direct down-conversion in phycobiliprotein PC645 via incoherent vibronic transport. In: *ArXiv e-prints* (Apr 2017). arXiv:1704.05449.

AT A GLANCE

FOUNDED: 2014

PROGRAM DIRECTOR: Edward H. Sargent, University of Toronto

FELLOWS, ADVISORS AND CIFAR AZRIELI GLOBAL SCHOLARS: 22

INSTITUTIONS REPRESENTED: 19, in 7 countries

FIELDS AND SUBFIELDS REPRESENTED: nanotechnology, including nanomaterials; physical and inorganic chemistry; polymer science; biophysics; chemical, molecular and quantum physics; optics; environmental engineering

MEETINGS: 2; in Montreal, Canada, and Cambridge, USA

RELEVANT KNOWLEDGE USERS: cleantech and biotech industrial sectors; economists; policy makers

PARTNER: Fonds de recherche du Québec — Nature et technologies

SUPPORTERS: The Arthur J.E. Child Foundation | Charles Hantho | Chisholm Thomson Family Foundation | Jerry and Geraldine Heffernan | Max Bell Foundation | Metcalf Foundation

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A collaborative project between Fellow **Gregory Scholes** (Princeton University) and Heffernan Director **Ted Sargent** (University of Toronto) led to a deeper understanding of charge transfer in novel solar cell materials and improved photovoltaics, and the discovery of ultrafast charge separation in low-dimensionality perovskites. This material has received a surge in interest owing to its greatly enhanced stability and high efficiencies. Through a Catalyst grant, postdoctoral fellow Madeline Elkins and PhD student Andrew Proppe found that perovskite materials exhibit the fastest rates of charge transfer ever observed in such systems. The study is expected to change how charge transfer in nanoparticle light harvesting systems is studied.

Fellows **Curtis Berlinguette** (University of British Columbia) and **Thomas Mallouk** (Pennsylvania State University) are working together to develop new device architectures for the reduction of carbon dioxide in flow cells. They developed electrolyzers that can convert gas-phase carbon dioxide to syngas (a chemical precursor to hydrocarbon liquid fuels). With this discovery, they are approaching the high current densities of commercial water electrolyzers, an important step forward towards the economical use of carbon dioxide for the synthesis of chemicals and fuels.

- Li YC et al. 2016. Electrolysis of CO₂ to Syngas in bipolar M] membrane-based electrochemical cells. ACS Energy Lett. 1: 1149-1153.

CIFAR fellows are providing expertise and leadership to shape the global energy research agenda. Deeply involved in developing a program for Mexico's Mission Innovation commitments on Clean Energy Materials, Fellow **Alán Aspuru-Guzik** (Harvard University) is holding an Energy Materials Innovation workshop in Mexico City on September 11-14, 2017. More than 50 scientists and experts in advanced theoretical and applied physical chemistry/materials sciences, advanced computing, machine learning and robotics will define research and development priorities and gaps, and propose opportunities for deeper collaborations. Fellows **Ted Sargent** (University of Toronto) and **Curtis Berlinguette** (University of British Columbia) are developing recommendations on behalf of the Canadian government for Mission Innovation's Converting Solar Energy challenge.

Other Notable Publications and Outputs

- Blaskovits JT, **Aspuru-Guzik A**, Leclerc M et al. 2016. A Study of the degree of fluorination in regioregular poly(3-hexylthiophene). Macromolecules. 50: 162-174.
- Ross MB, **Sargent EH**, Yang P et al. 2017. Tunable Cu Enrichment enables designer syngas Electrosynthesis from CO₂. J Am Chem Soc. Accepted (DOI: 10.1021/jacs.7b04892).
- Stott LA, **Warren JJ** et al. 2017. Lowering water oxidation overpotentials using the ionisable imidazole of copper(2-(2'-pyridyl)imidazole). Chem Commun. 53: 651-654.

IDEAS EXCHANGE

Program member **Gregory Scholes** (Princeton University) participated in a CIFAR-led plenary presentation at the Canadian Science Policy Conference in Ottawa. Titled Collaboration and Cooperation on the Challenge of Clean Energy: An International Perspective, the panel of global leaders from academia, government and industry explored the mechanisms that enable governments, the scientific community, and industry to work together to transform clean energy science and technology.

Program members also engaged in a discussion with global stakeholders in a CIFAR-led roundtable on the Future of Energy in Boston. The roundtable centred on three themes: future energy consumption and costs, future of energy harvesting and storage, and the role of policy in regulation and adoption.

GLOBAL ACADEMY

The program welcomed its first two CIFAR Azrieli Global Scholars in 2016/2017: **Gabriela Schlau-Cohen** (Massachusetts Institute of Technology) and **Jeffrey Warren** (Simon Fraser University). Both presented their latest research at the October 2016 program meeting.

In advance of the October meeting, trainees had an opportunity to present their work to program fellows, in addition to holding a poster session during the meeting to further engage fellows on their research.