Academic Outreach Workshop
Department of Chemistry & Chemical Biology
Harvard University

Summary

The goal of this one-day workshop is to create a forum of interaction between young researchers at the University of Puerto Rico, Rio Piedras, and faculty from the Department of Chemistry and Chemical Biology at Harvard University. The workshop will begin with a series of short talks describing frontier areas of each faculty's research. We will follow with a discussion of undergraduate and graduate research opportunities at Harvard. Students interested in specific areas will meet with individual faculty in breakout sessions to talk about research and career opportunities in chemistry and related areas.

Schedule

9:00 am	Welcome and Introduction
9:10 am	Quantum Information and Chemistry (Alán Aspuru-Guzik)
9:40 am	Energy and Chemistry (Theodore Betley)
10:10 am	Organic Chemistry and Medicine (Tobias Ritter)
10:40 am	Break
11:00 am	Photosynthesis (César Rodríguez-Rosario)
11:30 am	Biochemistry (Alan Saghatelian)
12:00 pm	Undergraduate Research Opportunities at Harvard
12:30 pm	Lunch
2:00 pm	Graduate School at Harvard and the Graduate School Application Process
3:00 pm	Breakout Sessions:
	Physical Chemistry (Alán Aspuru-Guzik, César Rodríguez-Rosario)
	Organic chemistry (Tobias Ritter)
	Inorganic and Nano (Theodore Betley)
	Chemical Biology (Alan Saghatelian)
4:30-5:00 pm	General Q&A and Wrap-up

Speaker Bios and Abstracts

Alán Aspuru-Guzik grew up in Mexico City and represented Mexico at the International Chemistry Olympiad. Alán studied Chemistry at the National Autonomous University of Mexico and graduated with the Gabino Barreda Medal of Honor in 1999. Alán obtained his Ph.D. in chemistry from UC Berkeley in 2004, and developed quantum Monte Carlo methods for molecular electronic structure. In 2005, he developed the first quantum algorithm for molecular quantum chemistry as a postdoctoral researcher in the group of Martin Head-Gordon. Since 2006, he has been leading a group of 12 researchers in the Department of Chemistry and Chemical Biology at Harvard University. Alán and his group work at the interface between quantum information and theoretical physical chemistry.

Research Interests: Quantum computation, molecular electronic structure, theory of open quantum systems, density functional theory, quantum Monte Carlo.

Quantum Information and Chemistry

The field of quantum information is a young new field that studies quantum mechanics as an information problem to answer fundamental questions such as: Can quantum systems be thought as computational devices? In my group, we study the potential use of quantum computers as simulators of chemical and physical systems, as well analyze photosynthetic energy transfer in terms of quantum information. In this talk, I will summarize some of our recent results in both areas.

Theodore Betley grew up in Plymouth, MI. He attended the University of Michigan from 1995-1999 and earned a degree in chemical engineering. During his undergraduate education, Ted held internship positions at Ford Motor Company, Exxon and IBM, as well as performing research in the Chemistry Department at Michigan. In 2000, Ted began his graduate studies in Inorganic Chemistry at the California Institute of Technology. In 2005, he completed his Ph.D. on chemistry related to iron mediated nitrogen reduction. From 2005 until 2007, Ted performed research related to water oxidation catalysis at MIT. In 2007, Ted began his current position at Harvard while his labs continue to develop and apply synthetic methodology for small molecule activation catalysis.

Chemistry's Impact on Energy and the Environment

What is the energy problem? How does continued use of fossil fuels impact the environment? Where will the future of energy be found? This talk will broadly put the energy problem into context and discuss a range of viable alternative energy sources as fossil fuel reserves diminish. A significant portion of time will be devoted towards making the connection between basic chemistry to cutting edge energy and environmental research.

Tobias Ritter was born in 1975 in Lubeck, Germany. He received his Master of Science from Braunschweig University, Germany in 1999 after studying in Braunschweig, Bordeaux, and Lausanne and a 1 year tenure at Stanford University with Professor Barry M. Trost. At Stanford Tobias' research dealt with palladium-catalyzed allylic alkylations and the synthesis of iridium and rhodium catalysts for olefin-isomerization. Subsequently, he moved to ETH Zurich for his doctoral studies in the group of Professor Erick M. Carreira on the total synthesis of the natural product Resiniferatoxin and new cholesterol absorption inhibitors. After obtaining his Ph.D. in 2004 Tobias started as a postdoctoral fellow at the California Institute of Technology with Professor Robert H. Grubbs. The focus of his work was the design, synthesis, and evaluation of new ruthenium-based olefin metathesis catalyst. Tobias began as an Assistant Professor in the Department of Chemistry and Chemical Biology at Harvard University in July 2006. His research program is based on synthetic organometallic and organic chemistry.

Chemistry in Medicine

How can Chemistry influence medicine? How can fundamental advances in chemistry impact other fields such as biomedical research? The talk will give a brief outline of the power of chemistry as a tool to develop new methods in biomedical research and present a case study how chemistry can have an immediate and lasting impact on molecular imaging.

César A. Rodríguez-Rosario studied Computer Engineering at UPR Mayagüez, while doing research in experimental solid state physics in UPR Rio Piedras. He received his Ph.D. in physics from The University of Texas in Austin. Currently, César is a Postdoctoral Fellow in the Department of Chemistry and Chemical Biology at Harvard University. His current theoretical research focuses on the role of quantum thermodynamics in photosynthesis.

Research interests: Quantum thermodynamics, quantum computation, quantum effects in biological systems, excitonic energy transfer and light harvesting complexes.

Quantum Effects in Photosynthesis (as part of the Outreach Conference, Friday January 23)

The process of absorption, transfer and conversion of energy in photosynthesis is extremely efficient. What can we learn from nature in order to fulfill our current energy needs? We review experiments and theories that demonstrate the important contribution of quantum effects to the efficiency of light harvesting complexes and energy transfer. This research lies at the intersection of biology, chemistry, physics, engineering and environmental science.

The Zeno Paradox: Quantum Measurement vs. Thermodynamics (Physics Department, Thursday January 22)

Observing something prevents it from changing. This is known as the quantum Zeno effect, in which repeated quantum mechanical measurements can slow down the evolution of a state. We discuss the relationship of the Zeno to thermodynamics. We derive a non-Markovian master equation to reconcile both.

Alan Saghatelian grew up in Glendale, CA. He attended UCLA from 1993-1997 and earned a degree in chemistry. While at UCLA, Alan worked with Professor Craig Merlic on the total synthesis of the Calphostin natural products using chromium carbene methodology. Later Alan traveled south to La Jolla, CA to attend graduate school at The Scripps Research Institute. There Alan developed supramolecular chemical systems capable of self-replication, DNA detection, and molecular computing in the laboratory of Professor M. Reza Ghadiri. During graduate school Alan's interest in biology began to peak. After receiving his Ph.D. in 2002, he worked with Professor Benjamin Cravatt on developing new global metabolite profiling methods. In 2006, Alan began his current position at Harvard as Assistant Professor of Chemistry. His lab continues to develop and apply global profiling approaches to the study of biological problems.

Abstract: The metabolism of physiological peptides is a complex process involving many proteins working in concert. Approaches that can provide insight into peptide regulation *in vivo* offer new possibilities for understanding and controlling these pathways. We reasoned that a mass spectrometry (MS)-based global peptide profiling approach would provide the most direct route for elucidating these metabolic pathways by identifying and quantifying changes in individual peptides. Indeed, profiling of kidney peptides from mice lacking dipeptidyl peptidase 4 (DPP4) revealed endogenous DPP4 substrates and also defined differences in peptide catabolism associated with the loss of this enzyme. Moreover, subsequent experiments using renal brush border membranes characterized a previously unrecognized pathway in the catabolism of proline-containing peptides that interlinks aminopeptidase and DPP4 activities. Together, these studies elucidate specific aspects of peptidase-regulated metabolism in the kidney and, more generally, highlight the utility of global peptide profiling for studying peptide metabolism *in vivo*.