Colorado State University's
Information Science and Technology Center (ISTeC)
presents two lectures by

Alán Aspuru-Guzik

Professor of Chemistry and Chemical Biology,
Department of Chemistry and Chemical
Biology, Harvard University

ISTeC Distinguished Lecture

In conjunction with the Chemistry Department, Computer Science Department, and Electrical and Computer Engineering Department

"Billions and Billions of Molecules: Exploring Chemical Space"

Thursday, February 19, 2015
Reception with refreshments: 10:30 am
Lecture: 11:00 am – 12:00 noon
Location: Grey Rock Room

•

Chemistry Department, Computer Science Department, and Electrical Engineering Department Special Seminar Sponsored by ISTeC

"Green Sulfur Bacteria: Nature's Photon Junkie"

Friday, February 20, 2015
Lecture: 4:00 pm – 5:00 pm
Location: Chemistry A101
Refreshments in B101E at 3:45 p.m.
Reception immediately following seminar in the Chemistry Lobby

ISTeC (Information Science and Technology Center) is a university-wide organization for promoting, facilitating, and enhancing CSU's research, education, and outreach activities pertaining to the design and innovative application of computer, communication, and information systems. For more information please see ISTeC.ColoState.EDU.

Abstracts

Billions and Billions of Molecules: Exploring Chemical Space

Many of the challenges of the twenty-first century are related to molecular processes such as the generation, transmission, and storage of clean energy, water purification and desalination. These transformations require a next generation of more efficient and ecologically-friendly materials. In the life sciences, we face similar challenges, for example drug-resistant bacterial strains require novel antibiotics. One of the paradigm shifts that the theoretical and experimental chemists needs to embrace is that of accelerated molecular discovery: The design cycles need to be sped up by the constant interaction of theoreticians and experimentalists, the use of high-throughput computational techniques, tools from machine learning and big data, and the development of public materials databases. I will describe three projects from my research group that aim to operate in this accelerated design cycle. First, I will describe our efforts on the Harvard Clean Energy Project (http://cleanenergy.harvard.edu), a search for materials for organic solar cells. I will continue by talking about our work on developing organic molecules for energy storage in flow batteries. Finally, I will describe our work towards the discovery of novel molecules for organic light-emitting diodes.

Green Sulfur Bacteria: Nature's Photon Junkie

Green Sulfur Bacteria is an early organism that can thrive at very low light conditions. It has an unique photosynthetic apparatus that transfers energy efficiently to the reaction center that is responsible to begin the chemical reactions to support life. The antenna complex, called Chlorosome is composed of up to a quarter million self-assembled bacteriochlorophylls. I will discuss our studies of the energy transfer in this system using a bottom-up approach that starts with atomistic simulations. I will end by discussing our work on the design ultrafast experiments that can help understand the dynamics of quantum systems, a technique called quantum process tomography that is commonly used in quantum information processing, and which we propose to employ in physical chemistry experiments as a tool to extract information from ultrafast spectra in a systematic manner.

Speaker Biography

Professor Alán Aspuru-Guzik is currently Professor of Chemistry and Chemical Biology at Harvard University, where he started his independent career in 2006 and promoted to Associate Professor in 2010 and Full Professor in 2013. Alán received his undergraduate degree in Chemistry from the National Autonomous University of Mexico (UNAM) in 1999. He received the Gabino Barreda Medal from UNAM, which prizes the top achiever in each field of study. After receiving his PhD in Physical Chemistry from the University of California, Berkeley in 2004, under Professor William A. Lester, Jr., he was a postdoctoral scholar in the group of Martin Head-Gordon at UC Berkeley from 2005-2006.

Professor Aspuru-Guzik carries out research at the interface of quantum information and chemistry. In particular, he is interested in the use of quantum computers and dedicated quantum simulators for chemical systems. He has studied the role of quantum coherence in excitonic energy transfer in photosynthetic complexes, and developed methodology for studying the spectroscopy of molecules in nanoscale environments. He and his group recently developed a density functional theory for open quantum systems. He leads the Clean Energy Project: a distributed computing effort for screening renewable energy materials.

In 2009, Professor Aspuru-Guzik recently received the DARPA Young Faculty Award, the Camille and Henry Dreyfus Teacher-Scholar award and the Sloan Research Fellowship. In 2010, he received the Everett-Mendelsson Graduate Mentoring Award and received the HP Outstanding Junior Faculty award by the Computers in Chemistry division of the American Chemical Society. In the same year, he was selected as a Top Innovator Under 35 by the Massachusetts Institute of Technology Technology Review magazine. In 2012, he was elected as a fellow of the American Physical Society and received the ACS Early Career Award in Theoretical Chemistry.

To arrange a meeting with the speaker, please contact Prof. Nancy Levinger, nancy.levinger@colostate.edu.