Resnick Young Investigators Symposium
Thursday, November 7, 2019 | 1:00 to 5:00 pm
Beckman Institute Auditorium | Caltech Campus

1:00   Opening Comments

1:15   Adam V. Subhas, PhD
       Assistant Scientist in Marine Chemistry and Geochemistry at Woods Hole
       Oceanographic Institution
       *The Marine Calcium Carbonate Cycle and its Role in Carbon Neutralization*

2:00   Samantha I. Johnson, PhD
       Computational Scientist at Pacific Northwest National Laboratory
       *Computational Understanding and Design of Catalysts for Energy Storage and Harvest*

2:45   Coffee Break

3:15   Prineha Narang, PhD
       Assistant Professor of Computational Materials Science at the John A. Paulson School of Engineering and Applied Sciences at Harvard University
       *Quantum Optical Control of Catalysis*

4:00   Raymond A. Weitekamp, PhD
       CEO and Founder of polySpectra, Inc.
       *A Tale of Two Technologies: Photonic Polymers from Publication to Product*

4:45   Closing Comments
Connecting to the Caltech Wireless Network

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Attendees may also join the 'eduroam' Network, if their Home Institution participates.

A recent feature in some web browsers called OCSP can prevent you from successfully connecting to the Caltech Conference Network. If this feature is available, it should be turned off.

We recommend using the Chrome Browser from Google as it does not use OCSP. If you do not have Chrome installed you may try to get a copy via USB, or do a search on how to Disable OCSP for your browser.

There are also some browser extensions available that will prevent the authentication screen from appearing such as 'HTTPS Everywhere'. These should be disabled for access.
Dr. Adam V. Subhas
Assistant Scientist in Marine Chemistry and Geochemistry at Woods Hole Oceanographic Institution

Adam was a biochemistry major at Haverford College, and in his senior year, realized that studying earth science could unite his love of the outdoors with his love of chemistry. After completing his PhD at Caltech with Jess Adkins, he moved to Woods Hole Oceanographic Institution as a postdoctoral scholar, working with the National Ocean Sciences Accelerator Mass Spectrometry laboratory.

In the spring of 2019, Adam transitioned to an Assistant Scientist position at Woods Hole in the department of Marine Chemistry and Geochemistry. He studies the cycling of carbon and alkalinity in open ocean and coastal environments, with the goal of understanding the timescales of carbon cycling, and buffering and neutralization of carbon dioxide, in the ocean.

The Marine Calcium Carbonate Cycle and its Role in Carbon Neutralization

Carbon dioxide has many paths through the Earth's biological and geological cycles. In this talk, I will present some recent work on understanding how carbon dioxide is neutralized through reaction with calcium carbonate minerals on several different time and space scales across the world's oceans. I will also touch upon the effects of the products of this reaction on ocean biogeochemistry, and the implications for using this process for global anthropogenic carbon sequestration.
Dr. Samantha I. Johnson
Computational Scientist at Pacific Northwest National Laboratory

Dr. Samantha Johnson is a Computational Scientist at Pacific Northwest National Laboratory. She studies molecular electrocatalysts for chemical energy storage and harvesting using theoretical and computational methods. In particular, she is interested in the role of a catalyst’s surroundings in its performance and behavior.

Dr. Johnson has a BS in chemical engineering from University of Colorado, Boulder. She received her PhD in materials science from California Institute of Technology in 2017 and was a postdoctoral researcher in the Center for Molecular Electro catalysis at Pacific Northwest National Laboratory.

She was a National Science Foundation Graduate Fellow and a Resnick Fellow during her graduate studies. She has received several awards for her research, including a Clean Energy Education and Empowerment (C3E) Poster Award and Best Poster at the Northwest Theoretical Chemistry Conference and a Department of Energy Team Science Award.
Computational Understanding and Design of Catalysts for Energy Storage and Harvest

Alternative energy sources, such as wind and solar, already contribute to our nation’s energy supply. In order to expand their reach, storage solutions for the energy produced must be found to account for these sources’ intermittency. Storing electrons in the chemical bonds of liquid fuels aids in two ways: it meets the challenge of storage and allows alternative energy to penetrate new energy sectors. However, storing these electrons in chemical bonds is often energetically expensive and involves movement of many protons and electrons, creating a complex process.

The challenge is to design catalysts that are efficient and selective for these reactions. My work uses computational chemistry tools to understand the properties of existing catalysts and use this knowledge to design new, more efficient catalysts. In this talk, I will discuss catalysts for hydrogen evolution, oxygen reduction, and ammonia oxidation.

Computational methods give atomistic insight into how these catalysts operate and provides mechanistic understanding for the underlaying processes. My results show some of the interesting and unanticipated paths these molecules take to store energy. I also show the ability for computational chemistry to predict new catalysts. I will also outline some of the challenges that computational chemistry faces, as well as some exciting new advances in the field.
Dr. Prineha Narang
Assistant Professor of Computational Materials Science at the John A. Paulson School of Engineering and Applied Sciences at Harvard University

Prineha Narang is an Assistant Professor at the John A. Paulson School of Engineering and Applied Sciences at Harvard University. Prior to joining the faculty, Prineha came to Harvard as a Ziff Environmental Fellow at the Harvard University Center for the Environment to explore the new field of excited state quantum materials and devices. She was also a Research Scholar in Condensed Matter Theory at the MIT Dept. of Physics, working on new theoretical methods to describe quantum interactions.

Prineha’s work has been recognized by many awards and special designations, including being named a Moore Inventor Fellow by the Gordon and Betty Moore Foundation for innovations in quantum science and technology, a CIFAR Azrieli Global Scholar by the Canadian Institute for Advanced Research, a Top Innovator by MIT Tech Review (MIT TR35), and a Young Scientist by the World Economic Forum in 2018. In 2017, she was named by Forbes Magazine on their “30under30” list for her work in atom-by-atom quantum engineering.

Prineha received her ScB in Materials Science from Drexel University and an MS and PhD in Applied Physics from the California Institute of Technology (Caltech), as a National Science Foundation Graduate Fellow and Resnick Sustainability Institute Fellow, where her work focused on understanding light-matter interactions in areas ranging from quantum plasmonics to nitride optoelectronics. Outside of science, she is an avid triathlete and runner.
Quantum Optical Control of Catalysis

Recent advances in nanophotonics, quantum optics, and low-dimensional materials have enabled precise control of light-matter interactions down to the nanoscale. Combining concepts from each of these fields, there is now an opportunity to create and manipulate photonic matter via strong coupling of molecules to the electromagnetic field. In the strong-coupling regime, the original constituents of the system lose their individual identity and hybrid quasi-particles of novel character are formed.

These hybridized states with mixed light-matter character can dramatically change the chemical landscape. For example, chemical reactions could be performed in optical high-quality factor cavities without the need to explicitly drive the system. Conversely, these optical cavities could be used to monitor the kinetic and thermodynamic properties of chemical reactions creating a new method of quantum chemical spectroscopy. Towards this goal, here we introduce a first principles framework to calculate strongly coupled light-matter systems. Specifically, we have shown a general time-dependent density-functional theory to study correlated electron, nuclear and photon interactions on the same quantized footing.

In our work we demonstrate the arising one-to-one correspondence in quantum-electrodynamical density-functional theory, introduce Kohn-Sham systems, and discuss possible routes for approximations to the emerging exchange-correlation potentials. We complement our theoretical formulation with the first ab initio calculation of a correlated electron-nuclear-photon system. This cavity-modulated molecular motion has the potential to alter and open new chemical reaction pathways as well as create new hybrid states of light and matter. Our work opens an important new avenue in introducing ab initio methods to the nascent field of collective strong vibrational light-matter interactions.
Dr. Raymond A. Weitekamp  
CEO and Founder of polySpectra, Inc.

Dr. Raymond Weitekamp is the founder and CEO of polySpectra, an advanced materials company on a mission to transform polymer 3D-printing from a prototyping aid into a production manufacturing tool. polySpectra's core technology is based on a discovery Raymond made during his PhD research at Caltech, where he worked in the laboratories of Prof. Bob Grubbs and Prof. Harry Atwater.

Raymond was a member of the founding cohort at Cyclotron Road, the groundbreaking hard technology innovation program at Lawrence Berkeley National Laboratory. Prior to Caltech, Raymond received an A.B. in Chemistry from Princeton University. Outside of polySpectra, he is a co-founder of Cypris Materials, a startup with the mission to reinvent color using paintable photonic crystals.

Cypris Materials spun out of a $5M ARPA-E award to manufacture inexpensive, paintable coatings to improve the energy efficiency of single pane windows. Additionally, Raymond curates PhDtoCEO.com, a website dedicated to helping scientists transition into entrepreneurship. He was recently recognized with the distinction of Forbes 30 under 30.
A Tale of Two Technologies: Photonic Polymers from Publication to Product

Dr. Weitekamp will share his experiences taking two Caltech inventions from his PhD thesis towards commercial products, each with wide-ranging implications for energy, manufacturing and sustainability.

First, Raymond will discuss the invention and commercialization of PhotoLithographic Olefin Metathesis Polymerization (PLOMP), via his startup company polySpectra. polySpectra has used PLOMP to develop a new family of photopolymers for additive manufacturing (aka 3D printing) - which enable new possibilities for the energy-efficient fabrication of high-performance polymer components for a wide variety of industrial applications. Additive manufacturing has the potential to unlock a new paradigm of distributed digital manufacturing, which is predicted to lower global energy demand by as much as 25%. However, this energy impact won't be realized without new chemistry to produce durable materials that are rugged enough for end-use applications.

Next, Raymond will share the story of Cypris Materials, a brand-new startup with the mission to reinvent color using paintable photonic crystals. Raymond will briefly share the history of this Caltech invention, as well as the current work towards developing spectrally-selective coatings to improve the energy efficiency of building envelopes. Specifically, the Cypris team has been working under the support of an ARPA-E grant to dramatically improve the energy efficiency of single-pane windows, which currently consume 4% of US Energy.