

Monday, June 1, 2020

Many-Body Interactions: From Quantum Mechanics to Force Fields

Judy Herzfeld, Brandeis University, "Cheap Electrons: Simulating Chemical Reactions with Semi-Classical Valence Electrons"
David Sherrill, Georgia Tech, "AI in Drug Design"

Tuesday, June 2, 2020

YAP/TAZ and TEAD: At the Crossroads of Cancer

Ann Marie Pendergast, Duke University, "TAZ/YAP signaling in Lung Cancer Brain Metastasis and the Response to Lung Injury"
Brian Rubin, Cleveland Clinic, "From the Bench to the Bedside with Epithelioid Hemangioendothelioma: a Vascular Cancer Driven by Hippo Pathway Dysregulation"

Wednesday, June 3, 2020

Physical Genomics and Transcriptional Engineering

Karen Reddy, Johns Hopkins University, "Measuring and Manipulating the 3D Genome"
Vadim Backman, Northwestern University, "Understanding the 'Operating System' of the Genome: the Structure and Function of Chromatin Packing"

Thursday, June 4, 2020

Nonlinear Optics

Sylvie Roke, Swiss Federal Institute of Technology in Lausanne, "A water window on membrane biochemistry"
Alex Benderskii, University of Southern California, "Asymmetric Response of Interfacial Water to the Applied Electric Field"

Friday, June 5th, 2020

Quinary Interactions: Structure, Dynamics, Function

Martin Gruebele, University of Illinois, "Quinary Interactions: Proteins, Viral Capsids, and Other Things that Assemble and Disassemble Inside Cells"
Margaret Johnson, Johns Hopkins University, "Exploiting 3D to 2D Localization to Control Protein Self-assembly"
Rigoberto Hernandez, Johns Hopkins University, "Nanoscale Models, Macroscale Impacts"

Monday, June 8, 2020

Active Matter

Tom Solomon, Bucknell University, "Swimming Bacteria in Fluid Flows: Invariant Manifolds and One-way Barriers"
Daniel Beller, University of California, Merced, "Active Liquid Crystals and their Topological Defect Loops"

Tuesday, June 9, 2020

Nuclear Pore Complexes and Smart Polymers

Anton Zilman, University of Toronto, "Nuclear Pore Complex: Simple Physics of a Complex Biomachine"
Tijana Talisman, City of Hope Comprehensive Cancer Center, "Applying Quantitative Single Molecule Localization Microscopy to Probe the Mechanism of Nucleocytoplasmic Transport"

Wednesday, June 10, 2020

#ShutdownAcademia #ShutdownSTEM

No webinar today. We will paused our work here at TSRC and rescheduled our lecturers that were set to present today, joining the academic world in a global effort that aims to "transition to a lifelong commitment of actions to eradicate anti-Black racism in academia and STEM."

Thursday, June 11, 2020

Phase Separation in Biology and Disease

Richard Kriwacki, St. Jude Children's Research Hospital, "Evolving Perspectives on the Role of Phase Separation in Nucleolar Structure and Function"
Shasha Chong, University of California, Berkeley, "Illuminating the Dark Proteome that Regulates Gene Transcription by Live-cell Single-molecule Imaging"

Friday, June 12, 2020

Interfacial Molecular and Electronic Structure and Dynamics

Carlos Baiz, University of Texas at Austin, "Dynamics at Heterogeneous Interfaces: Ultrafast Spectroscopy of Soap"
Julianne Gibbs, The University of Alberta, "Deconvoluting the Stern Layer from the Diffuse Layer at Aqueous Interfaces with Nonlinear Optical Spectroscopy"

Monday, June 15, 2020

Spectroscopy & Dynamics on Multiple Potential Surfaces

Chris Johnson, Stony Brook University, "From Molecules to Clouds: How do Atmospheric Particles Form from Thin Air?"

Tuesday, June 16, 2020

Molecular Chemistry in Electrochemical Energy Storage

Matthew T. McDowell, Georgia Tech, "Watching Batteries Work: Understanding Reaction Mechanisms in Next-Generation Battery Materials"

Kimberly See, Caltech, "Going Beyond Conventional Charge Storage Mechanisms: Multielectron Redox Processes for High Capacity Cathodes"

Wednesday, June 17, 2020

Ab-initio Design and Control of Quantum Materials

Jeremy Levy, University of Pittsburgh, "1D Quantum Simulation with LaAlO₃/SrTiO₃ Nanostructures"

Prineha Narang, Harvard University, "Predicting Dynamics and Decoherence in Quantum Systems"

Thursday, June 18, 2020

Challenges in Large-Scale Biomolecular Simulations

Jeremy C. Smith, Oak Ridge National Laboratory, "How to Quickly Find a Cure for COVID-19"

Rommie Amaro, University of California, San Diego, "Computational Microscopy of SARS-CoV-2"

Friday, June 19, 2020

Advances of Multidimensional Vibrational Spectroscopy in Water, Biology and Materials Science

Lu Wang, Rutgers University, "Modeling the Vibrational Spectra of Nucleic Acids"

Wei Xiong, University of California, San Diego, "Intermolecular Vibrational Energy Transfer Enabled by Strong Coupling – A COVID-19 Resolution for Molecules"

Monday, June 22, 2020

New Experimental and Theoretical Developments in High Entropy Materials

Irene Beyerlein, University of California, Santa Barbara, "Dislocation Dynamics in Refractory Multi-Principal Element Alloys"

Stefano Curtarolo, Duke University, "Data, Disorder and Materials"

Tuesday, June 23, 2020

Enhanced Functionalities in 4 and 5d Transition Metal Compounds from Large Spin-Orbit Coupling

Valery Kiryukhin, Rutgers University, "Imaging Antiferromagnetic Domains"

Sobhit Singh, Rutgers University, "Theoretical Proposals for Realization of Weyltronics in MoTe₂"

Wednesday, June 24, 2020

Single Molecule Workshop: Theory Meets Experiment

Matthew Comstock, Michigan State University, "Watching human telomerase in action with high resolution tweezers and fluorescence"

Sabrina Leslie, McGill University, "Single-molecule Insights for Drug Discovery and Development: the Next Level of Resolution"

Thursday, June 25, 2020

Complexity in the Chemistry and Physics of Lipid Membranes

John Katsaras, Oak Ridge National Laboratory, "Deuterium, Neutrons and Biological Membranes"

Anne Kenworthy, University of Virginia, "Building Functional Membrane Nanodomains"

Friday, June 26, 2020

Challenges in RNA Structural Modeling and Design

Joint panel discussion on RNA and COVID-19

Tamar Schlick, New York University, "Covid-19 and RNA Modeling Challenges"

Samuela Pasquali, Laboratory of Theoretical Biology, University of Paris, "Modeling Energy Landscapes of Non-coding RNAs with Applications to G-quadplexes and the Regulatory RNA 7SK"

Monday, June 29, 2020

Electronic and Magnetic Properties of Chiral Structures and Their Assemblies

Vladimiro Mujica, Arizona State University, "The Chiral Induced Spin Selectivity- What it is and Proposed Mechanism"

Ron Naaman, Weizmann Institute of Science, "The Chiral Induced Spin Selectivity- How it is Manifested in Life and how it can be Utilized"

Tuesday, June 30, 2020

Hydrophobicity: From Theory, to Simulation, to Experiment

Paul Cremer, Pennsylvania State University, "Real-Time Continuous Sensing of SARS-CoV-2"

Gul Zerze, Princeton University, "Liquid-Liquid Critical Point in Realistic Models of Water"

Wednesday, July 1, 2020

Molecular Rotors, Motors & Switches

Alberto Credi, University of Bologna, "Artificial Molecular Machines: From Laboratory Curiosities to the Nobel Prize in Chemistry"

Angelique Louie, University of California, Davis, "(Don't) See the Light: Molecular Babel Fish for Optically Triggered Non-optical Imaging"

Thursday, July 2, 2020

No Talks

Friday, July 3, 2020

No Talks

Monday, July 6, 2020

International Conferences on Computational and Mathematical Medicine

Jayajit Das, Nationwide Children's Hospital, "Quantitative Modeling of Lymphocyte Signaling and Activation"

Paola Malerba, Nationwide Children's Hospital, "Sleep to Remember: Mechanisms Linking Sleep Oscillations to Memory Consolidation"

Tuesday, July 7, 2020

The Molecular Underpinnings of Astrophysics

Marissa Weichman, Princeton University, "Spectroscopy, Optical Pumping, and Collisional Energy Transfer of Cold Buckminsterfullerene"

David Neufeld, Johns Hopkins University, "Discovery of the Helium Hydride Cation (HeH⁺) in an Astrophysical Nebula"

Wednesday, July 8, 2020

Nucleic Acid Chemistry

Kristin Koutmou, University of Michigan, "Molecular Level Consequences of mRNA Modification on Translation"

Sheila David, University of California, Davis, "Dare to Repair: From DNA Chemistry to Cancer and Back Again"

Thursday, July 9, 2020

Proton Transfer in Biology

Marilyn Gunner, The City College of New York, "Powering the Cell: Mechanisms of Proton Shuttling in Oxidative Respiration"

Thomas Moore, Arizona State University, "Powering the Future: Proton Shuttling Captured in Artificial Photosynthesis"

Friday, July 10, 2020

Breaking and Making Bonds with Light

Steven Lopez, Northeastern University, "In Silico Photodynamics Towards Energy-dense Materials"

Monday, July 13, 2020

Activation of Small Molecules

Jenny Yang, University of California, Irvine, "Bio-inspired Catalysis for Renewable Fuels"

Paul Walton, University of York, UK, "Only Use O₂ When it's Needed: How Copper-containing LPMOs Control Oxygen Activation"

Tuesday, July 14, 2020

Condensed Phase Dynamics

Nandini Ananth, Cornell University, "Quantum Dynamics from Classical Trajectories"

Garnet Chan, Caltech, "Quantum Simulation of Molecules and Materials on Quantum and Classical Computers"

Wednesday, July 15, 2020

Interfacial Chemistry and Charge Transfer for Energy Storage and Conversion

Veronica Augustyn, NC State University, "Electrochemistry of Hydrated Metal Oxides: From Fundamental Understanding to High Power Energy Storage"

Keith Stevenson, Skoltech, "Beyond Lithium Ion Batteries: Challenges and Opportunities"

Thursday, July 16, 2020

Electronic and Structural Dynamics in Hybrid Perovskites: Theory & Experiment

Amanda Neukirch, Center for Nonlinear Studies, Los Alamos National Laboratory, "Catching the Sun and Beyond: The Development of Perovskites for Efficient Photovoltaic and Detector Applications"

Andrew Rappe, University of Pennsylvania, "Bridging Computers and Experimental Bench: Making More Efficient and Mechanically Robust Perovskite Optoelectronic Devices"

Friday, July 17, 2020

Quantum Frontiers in Molecular Science

Alexandra Olaya-Castro, University College London, "Vibronic Coherence and Synchronisation of Molecular Motions"

Thomas Weinacht, Stony Brook University, "Time-Resolved Spectroscopy of Molecular Dynamics: Comparing Different Approaches"

Monday, July 20, 2020

XXVth International Symposium on the Jahn-Teller Effect

Horst Koeppel, University of Heidelberg, "Multi-state Jahn-Teller Intersections: Nonadiabatic Dynamics and their Detection in Real Time"

Spiridoula Matsika, Temple University, "Conical Intersections and Non Adiabatic Dynamics in Conjugated Molecules"

Tuesday, July 21, 2020

Multi-scale Quantum Mechanical Analysis of Condensed Phase Systems

Nir Goldman, Lawrence Livermore National Laboratory, "Elucidating Prebiotic Chemistry Under Impact Conditions"

Aurora Clark, Washington State University, "Structural and Dynamic Topology of Complex Solutions"

Wednesday, July 22, 2020

Accelerating Reaction Discovery

Sarah Wengryniuk, Temple University, "Novel Umpolung Strategies Enabled by Hypervalent Iodine Reagents"

Sidney Wilkerson-Hill, University of North Carolina at Chapel Hill, "Synthetic Strategies Inspired by Complex Natural Products"

Thursday, July 23, 2020

Information Engines at the Frontiers of Nanoscale Thermodynamics

Jim Crutchfield, University of California, Davis, "Demonology: The Curious Role of Intelligence in Physics and Biology"

Friday, July 24, 2020

Iron at the Air-Sea Interface

Nicholas Meskhidze, NC State University, "Atmospheric Sources of Iron to the Global Ocean and Possible Climate Effects"

Hind A. Al-Abadleh, Wilfrid Laurier University, "Atmospheric Chemistry of Iron with Organics Relevant to Cloud Droplets and Wet Aerosols"

Monday, July 27, 2020

Optimizing Thermodynamic Systems

Chris Essex, Western University, Canada, "Slow Time"

Ty Roach, Hawaii Institute of Marine Biology, "Wholome Thermodynamic Feedback: The Role of Bacterial Biophysics in Ecological Processes"

Tuesday, July 28, 2020

Machine Learning and Informatics for Chemistry and Materials

TBD

Wednesday, July 29, 2020

Frontiers in Metabolomics

Clary Clish, Broad Institute, "Application of Metabolomics to Find Early Indicators of Disease in Human Cohorts"

David Wishart, University of Alberta, "In Silico Metabolomics: Using Machine Learning to Identify the Dark Matter of the Metabolome"

Thursday, July 30, 2020

Developments in QM/MM and Embedding models for Photochemical and Electron Transfer Processes

Ksenia Bravaya, Boston University, "Simulating Redox Potentials of Biomolecules: the Role of Environment Polarization"

Yihan Shao, The University of Oklahoma, "Energy Densities in the Linear-Response and Real-Time Time-Dependent Density Functional Theory Calculations"

Friday, July 31, 2020

Biomolecular Interactions in the Cellular Environments

Bethany Buck-Koehntop, University of Utah

Scott Showalter, Penn State University, "Disordered Proteins in Control: Regulating Transcription in Eukaryotes"

Monday, August 3, 2020

Epithelial Physiology and Cell Biology

Arohan (Ro) Subramanya, University of Pittsburgh, "Control of Cell Volume via Phase Separation"

My Helms, University of Utah

Tuesday, August 4, 2020

New Insights Into Gas-Phase Atmospheric Chemistry

Brian McDonald, NOAA, "Insights into Urban Air Chemistry: Before and During the COVID-19 Pandemic"

Wednesday, August 5, 2020

Platinum Group Metal-free Electrocatalysts: Small Molecules Activation and Conversion

Paul Kenis, University of Illinois, "CO₂ Reduction Technologies and Their Impact"

Plamen Atanassov, University of California, Irvine, "The Importance of Hydrogen in Transportation and Mobility"

Thursday, August 6, 2020

Chromatin Structure and Dynamics

Yamini Dalal, National Institutes of Health, "Bungee Jumping into Chromosomes: Mapping Elasticity of Fragile Sites in the Human Genome"

Lucy Bai, Pennsylvania State University, "Chemically Induced Chromosomal Interaction (CICI): A New Tool to Study Chromosome Dynamics and Its Biological Roles"

Friday, August 7, 2020

Ions in Solution: Biology, Energy, and Environment

Katie Maerzke, Los Alamos National Laboratory, "First Principles Simulations of CuCl in High Temperature Water Vapor"

Susan Rempe, Sandia National Laboratories, "How to Capture Carbon Inexpensively"

Monday, August 10, 2020

Organic Bioelectronics: Tackling the Mixed Conduction Challenge

George Malliaras, University of Cambridge, UK, "Are Conducting Polymer Electrodes Capacitive or Faradaic?"

Luisa Torsi, University of Bari, Italy, "Single Molecule Marker Detection with a Large Transistor"

Tuesday, August 11, 2020

Energy Landscapes: Structure, Dynamics and Exploration Algorithms

David Leitner, University of Nevada, "Fluctuations and Reaction Dynamics on Biomolecule Energy Landscapes"

Aurora Clark, Washington State University, "Descriptors of Energy Landscapes using Topological Data Analysis"

Christian Schoen, Max Planck Institute

Wednesday, August 12, 2020

Spatio-Temporal Dynamics of Excitons: Bridging the Gap Between Quantum Mechanics and Applications

Carlos Silva, Georgia Tech, "Exciton Polarons in Hybrid Organic-Inorganic Semiconductors"

Dorthe Eisele, The City College of New York, "Robust Frenkel Excitons Despite Extreme Heat Stress: Stable Supramolecular Nanocomposites via Tunable, Cage-like Scaffold Design"

Thursday, August 13, 2020

Coarse-Grained Modeling of Structure and Dynamics of Biomacromolecules

George Rose, Johns Hopkins University, "Protein Folding: Seeing is Deceiving"

Banu Ozkan, Arizona State University, "Protein Function and Dynamics Through the Lens of Evolution"

Friday, August 14, 2020

Plasticity in Biological Organization

Liam Holt, New York University

Lucia Strader, Duke University