

Molecular Conduction & Sensing Workshop
July 18-20, 2007
Purdue University, Burton Morgan Building, Room 121

Wednesday, July 18

- 8:30-10:00** **Registration & Breakfast – Burton Morgan Building**
- 10:10 Welcome – Dave Janes
- 10:30 Misha Galperin, Northwestern University
 “Simple Models for Molecular Transport Junctions”
- 10:55 Ajit Mahapatro, Purdue University
 “Metal-Molecule-Metal Junctions with Redox-Active and Substituted OPE Molecules”
- 11:20 Chad Risko, Northwestern University
 “Impact of Charge Injection Barrier on Conductance”
- 11:45** **Lunch – Birck Nanotechnology Building - Atrium**
- 1:00 Mark Hersam, Northwestern University
 “Submolecular Resolution Characterization of Organically Functionalized Silicon Surfaces”
- 1:25 Christina Hacker, National Institute of Standards and Technology
 “Metal-Molecule Interface Reactions for Silicon-Based Molecular Electronic Devices”
- 1:50 Adina Scott, Purdue University
 “Contact Effects in Metal-Molecule-Silicon Devices”
- 2:15 Nadine Gergel-Hackett, National Institute of Standards and Technology
 “Silicon-based Molecular Electronic Devices For Hybrid Molecular Device/CMOS Circuits”
- 2:40** **Break – Burton Morgan Café**
- 3:10 Ron Reifenberger, Purdue University
 “Aryl Diazonium Molecules Assembled on Si(111): STM I(V) and AFM F(z)”
- 3:35 Richard McCreery, University of Alberta
 “Conductance Switching in Fluorene/TiO₂ Molecular Heterojunctions”
- 4:00 Bhaskaran Muralidharan, Purdue University
 “Physics of Contact Induced Current Assymetry in Transport Through Molecules”
- 4:25 Kamil Walczak, University of Virginia
 “Modeling Molecule-Assisted Transport in Nanotransistors”
- 4:50** **Poster Session – Birck Nanotechnology Building - Atrium**
- David Andrews, Northwestern University
 “Molecular Electronic Junctions”
- Kanhayalal Baheti, Berkeley
 “Thermopower of Single Molecule Junctions”
- Kirk Bevan, Purdue University *“First-Principles Analysis of STM Image Heights of Styrene on Si(100)”*
- Dr. Thorsten Hansen, Northwestern University
 “Molecular Wires – A Fock Space Approach”

Zhifeng Huang, Arizona State University
“Stability of Single Molecule Junctions Formed via Au-Thiol Contact”

Takuya Masuda, Arizona State University
“Thermal Activated Electron Transport in Single Molecules”

Pradeep Nair, Purdue University
“Physics of Nanobiosensors”

Kumar Parimal, Indiana University
“Design, Synthesis and Electronic Properties of Redox Active, Mixed-Valence Molecular Wires”

Hassan Raza, Cornell University
“Si Surface States”

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“Dephasing and Molecular Electronics”

Amanda Schuckman, Hunter College of the City University of New York
“Surface Organization of Thiol Tethered Tri-Pyridylporphyrin Derivatives on Gold”

Gemma Solomon, Northwestern University – *“Symmetry, Chirality and Geometry: Chemical Variation and the Effects on Molecular Conductance”*

Edward Witlicki, Indiana University
“Studies of Redox-Active Molecular Wires Self-Assembled Onto Gold Surfaces”

Thursday, July 19

8:00 ***Continental Breakfast – Burton Morgan Café***

8:30 James Batteas, Texas A&M University
“Fabrication of Nanoscale Test Arrays for Studies of Molecular Conduction”

8:55 James Kushmerick, National Institute of Standards and Technology
“Electronic and Vibronic Spectroscopy of Molecular Junctions”

9:20 Supriyo Datta, Purdue University
“Molecular Electronics and the Bottom-Up View of Electronic Conduction”

10:05 ***Break – Burton Morgan Café***

10:35 Sina Yeganeh, Northwestern University
“Modeling Charging-based Switching in Molecular Transport Junctions”

11:00 Mark Hybertsen, Brookhaven National Lab/Columbia University
“Exploring Trends in Conductance for Well-Defined Single Molecule Circuits”

11:25 Fang Chen, Arizona State University
“Tuning the Conductance of Single Molecules by Chemical and Electrochemical Modification”

11:50 ***Lunch – Birck Nanotechnology Building - Atrium***

- 1:00 Nathan Swami, University of Virginia
“Enhancing Surface Binding Kinetics Through Electrodeless Dielectrophoresis”
- 1:25 Samir Iqbal, Purdue University
“Silicon Based nanoporre Sensors for Detection of DNA Molecules”
- 1:50 Scott Crittenden, University of South Carolina
“Electrogenic Bacteria: Microbial Fuel Cells/Chemoelectric Biosensors”
- 2:15 Michael Garcia, Duke University
“Impact of Porphyrin Functional Groups on InAs Gas Sensors”
- 2:40 Steve Howell, Sandia National Laboratories
“Nano-Enabled Smart Chemiresistors for Improved Chemical Sensing”
- 3:05 Break – Burton Morgan Café**
- 3:35 Su-Ying Quek, Berkeley
“Amine-Gold Linked Single-Molecule Junctions: First-Principles Calculations and Comparison to Experiment”
- 4:00 Jeff Neaton, Lawrence Berkeley National Lab
“Electronic Level Alignment at Metal-Molecule Contacts with a GW Approach”
- 4:25 Tour of the Birck Nanotechnology Center**

Friday, July 20

- 8:00 Continental Breakfast – Burton Morgan Café**
- 8:30 Yongqiang Xue, State University of New York
“A Quantum Open Systems Approach to Molecular-Scale Devices”
- 8:55 Amy Walker, Washington University in St. Louis
“New Methods for metal Deposition on Alkanethiol Self Assembled Monolayers: Towards Molecular Electronic Circuitry”
- 9:20 Garrett Rose, Polytechnic University
“Modeling and Design Approaches of Emerging Nanoelectronic Circuits and Systems”
- 9:45 Break – Burton Morgan Café**
- 10:40 Bruce Hinds, University of Kentucky
“Dramatic Resistance Increase and Magnetic Ordering with Magnetic Molecular Electrodes”
- 11:05 Andrei Sokolov, University of Nebraska
“Ballistic Anisotropic Magnetoresistance in Electrodeposited Co Nanocontacts”
- 11:30 Vladimiro Mujica, Northwestern University
“A Mean-Field Model for Magnetism in Gold Nanoparticles”
- 11:55 TBD
- 12:20 Wrap-Up
- 12:30 Adjourn

Organizers:

Chad Risko (Northwestern)

Nadine Gergel-Hackett (NIST)

David Janes (Purdue)

Mark Hybertsen (Brookhaven/Columbia)