PROGRAM

MOLECULAR-SCALE ELECTRONICS VII

January 23 – 26, 2005

Bahia Resort Hotel
998 West Mission Bay Drive
San Diego, California 92109
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Conference Chair

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ECI

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Six MetroTech Center -- Brooklyn, NY 11201
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Sunday, January 23. 2005

16:00 – 18:00 Conference Registration (Del Mar)

18:00 – 19:30 *Opening Dinner (Del Mar)*

19:30 – 20:00 Introduction and Opening Remarks: R. Shashidhar and M. Stone

20:00 – 22:00 **Special Session in Honor of Ari Aviram**
(Chair: Mark Ratner)

Invited Speakers

Switching with a Molecule in the 80s
Christian Joachim
GNS-CEMES/CNRS

Noel Hush
University of Sydney

Tunneling Through Molecules: Zen Barrier with No Gate
J. Gimzewski

Mark Reed
Yale University

Nongjian Tao
Arizona State University

Pomerantz
IBM

22:00 – 23:00 *Reception*

NOTES

- **All technical sessions will be held in Bay E Room (3rd Floor Main Bldg. North Entrance).**
- **All poster sessions will be in Bay E.**
- **Please observe "No Smoking" at ECI technical sessions, meals and social hours.**
- **Speakers should allow time at the end of their presentation for questions and discussion.**
- **Please silence your cell phone during technical sessions.**

Monday, January 24, 2005

07:00 – 08:00 *Breakfast (Del Mar)*

Session 1: Materials and Chemistry
(Chair: Marcel Mayor)

08:00 – 08:30 *TBA*
James Tour
Rice University

08:30 – 09:00 *Functional p-Electron Materials for Nanoelectronics*
Peter Bäuerle
University of Ulm

09:00 – 09:30 *Supramolecular Engineering at Surfaces: Control of Matter at the Nanoscale*
J.V. Barth
University of British Columbia

09:30 – 10:00 *Towards Self-Assembling Circuit Boards for Molecular Electronics*
Marya Lieberman
University of Notre Dame

10:00 – 10:30 *TBA*
David Allara
Pennsylvania State University

10:30 – 11:00 *Coffee Break*

Session 2: Materials and Chemistry (continued)
(Chair: Theresa Mayer)

11:00 – 11:30 *Organic Molecules in Electronic Devices: Single Molecule, Single Electron Transistors and Self-Assembled Circuitry*
Thomas Bjornholm
University of Copenhagen

11:30 – 12:00 *Red, Green, Blue and White Electroluminescent Materials*
Luisa De Cola
University of Amsterdam

12:00 – 12:30 *Photoswitching of Structure/Function Relationships in Materials Science*
Neil Branda
Quebec, Canada

Monday, January 24, 2005 (continued)

12:30 – 13:00 *Pyridine on Si(100) and H-Si(100) -- STM Observation of Dative Bonded Adducts*
Greg Lopinski
University of Quebec

13:00 – 13:30 *In Situ Sensing of Cytochrome C Molecules Using Single-Walled Carbon Nanotubes with Passivated Source and Drain Electrodes*
Islamshan Amlani
Motorola, Inc.

13:30 – 14:30 *Lunch (Del Mar)*

Session 3: Theory
(Chair: Noel Hush)

14:30 – 15:00 *Three Key Factors Responsible for the Failure of A Priori Computational Schemes to Describe Through-Molecule Conductivity*
Jeffrey R. Reimers
University of Sydney

15:00 – 15:30 *Schottky Barrier Concepts Applied to Metal-Molecule Interfaces*
Raymond T. Tung
Brooklyn College of City University of New York

15:30 – 16:00 *An Ab-Initio Analysis of Electron Transport Characteristics for the Au(111) -Octane Dithiol- Au(111) System: Electrode Spacing and Coverage Effects*
Neeti Kapur
University of Virginia

16:00 – 16:30 *Approximated Quantum Chemistry Models for the Study of Molecular Conductance: Towards A Systematic Validation*
Carlos A. Gonzalez
National Institute of Standards and Technology

16:30 – 17:00 *Coffee Break*

Monday, January 24, 2005 (continued)

Session 4: Theory (continued)
(Chair: Jeffrey Reimers)

17:00 – 17:30 *Molecular Wires From 1,3- And 1,4-Disila/Germa/Stannabicyclo [K.L.M] Alkane Monomers (K, L, M = 1 or 2): Interesting Targets For Molecular Electronics?*
Henrik Ottosson
Uppsala University

17:30 – 18:00 *Overcoming the Constraints of Modeling: Obtaining Chemical Sensitviity in Single Molecule Conduction Calculations*
Gemma C. Solomon
University of Sydney

18:00 – 18:30 *Theoretical Approach for Transport Properties of Porphyrin and Phthalocyanine Oligomers*
Hiroshi Mizuseki
Tohoku University

18:30 – 19:00 *Combining Current and Shot Noise: Towards Full Characterization of Molecular Nanojunctions*
Matthias H. Hettler
Forschungszentrum Karlsruhe, INT

19:00 – 20:30 *Dinner (William D. Evans)*

20:30 – 22:00 Posters and *Social Hour (Bay E)*

Tuesday, January 25, 2005

07:00 – 08:30 *Breakfast (Del Mar)*

Session 5: Single Molecule Characterization
(Chair: Paul Weiss)

08:00 – 8:30 *TBA*
Heiko Weber
Forschungszentrum Karlsruhe, INT

08:30 – 09:00 *Towards Monomolecular Computing: Single Molecular Devices*
Andre Gourdon
CNRS NanoSciences Group CEMES

09:00 – 9:30 *TBA*
N. J. Tao
Arizona State University

09:30 – 10:00 *Voltage Controlled Molecular Conductance Switching*
Amy Szuchmacher Blum
Naval Research Laboratory

10:00 – 10:30 *Coffee Break*

Session 6: Metal/ Nonmetal Molecule Contacts
(Chair: James Ellenbogen)

10:30 – 11:00 *TBA*
David Janes
Purdue University

11:00 – 11:30 *Variable Temperature Charge Transport Measurements of Molecule-Silicon Junctions Using Ultra-High Vacuum Scanning Tunneling Microscopy*
Nathan L. Yoder
Northwestern University

11:30 – 12:00 *Electrical Characterization of Top-Metal/Molecule Interactions in Molecular Electronic Devices*
Curt A. Richter
National Institute of Standards and Technology

12:00 – 12:30 *The Structural Influence of Bis(Terpyridinyl) Transition Metal Complexes on Charge Storage Behavior of A Nanowire Transistor*
Wendy Fan
NASA Ames Research Center

Tuesday, January 25, 2005 (continued)

12:30 – 13:30 *Lunch (Del Mar)*

Session 7: Molecular Switching
(Chair: Ari Aviram)

13:30 – 14:00 *TBA*
Paul Weiss
Pennsylvania State University

14:00 – 14:30 *Understanding Charge Transport In Molecular Electronics*
James Kushmerick
Naval Research Laboratory

14:30 – 15:00 *Molecular Electromechanical Switching from Electronic Devices to the Solution Phase*
Amar H. Flood
University of California at Los Angeles

15:00 – 15:30 *Understanding Negative Differential Resistance/Switching with Memory Observed from the Nitro Molecule*
N. Gergel
University of Virginia

15:30 – 16:00 *Coffee Break*

Session 8: Devices and Architecture
(Chair: Christian Joachim)

16:00 – 16:30 *Integration of Molecular Electronic Devices and Architectures*
Paul D. Franzon
North Carolina State University

16:30 – 17:00 *System Simulations and Analyses for Nanoprocessors Integrated on the Molecular Scale*
James C. Ellenbogen
The MITRE Corporation

17:00 – 17:30 *Multilevel Molecular Memory*
Chongwu Zhou
University of Southern California

17:30 – 18:00 *Towards Quantum Computing Using Mixed Valence Molecules*
Jacques Bonvoisin
CNRD/CEMES-GNS

<u>Tuesday, January 25, 2005</u> (continued)

18:00 – 18:30	*The Molecular Crossbar Latch: A Key enabler for Nanoscale Computers* Duncan Stewart Hewlett-Packard Laboratories
18:30 – 19:00	*Intrinsic Electron Conduction Mechanisms in Molecules* David Routenberg Yale University
19:00 – 20:00	Poster Session with *Social Hour (Bay E)*
20:00 – 21:30	*Dinner (Del Mar)*

Wednesday, January 26, 2005

07:00 – 08:30 *Breakfast (Del Mar)*

Session 9: Devices and Architecture
(Chair: Mark Reed)

08:00 – 08:30 *From Classical to Quantum Mono-Molecular Electronics*
Christian Joachim
GNS-CEMES/CNRS

08:30 – 09:00 *Carbon Nanotube Electronics And Optoelectronics*
Jia Chen
IBM T.J. Watson Research Center

09:00 – 09:30 *Silicon Contacts: A New Playground for Molecular Electronics?*
Avik W. Ghosh
Purdue University

09:30 – 10:00 *Programmable Logic Using Molecular Devices in a Three Dimensional Architecture*
Garrett S. Rose
University of Virginia

10:00 – 10:30 *Ballistic Emission Electron Microscopy Studies of Au-Octanedithiol-GaAs Diodes*
Julia W. P. Hsu
Sandia National Laboratories

10:30 – 11:00 *Coffee Break*

Session 10: Bioelectronics
(Chair: Heiko Weber)

11:00 – 11:30 *A Molecular Memory Device Using a Plant Virus as a Scaffold*
Banahalli R. Ratna
Naval Research Laboratory

11:30 – 12:00 *Ambipolar Charge Injection and Transport in a Single Organic Monolayer Island*
Dominique Vuillaume
IEMN-CNRS

12:00 – 12:30 *Direct Conductance Measurements of Single DNA Duplexes*
Joshua Hihath
Arizona State University

Wednesday, January 26, 2005 (continued)

12:30 – 13:00 *Hysteresis and Negative Differential Resistance: A Polaron Model*
Michael Galperin
Northwestern University

13:00 – 14:00 *Lunch (Pond – outside)*

Session 11: Devices and Their Characterization
(Chair: A. Gourdon)

14:00 – 14:30 *TB-LMTO Method for Nonequilibrium Electron Transport in Nanosystems*
Sergey Faleev
Sandia National Laboratories

14:30 – 15:00 *Implementation of Molecular Logic Gates with Array Device Having Nano-Via-Holes*
Hyoyoung Lee
Electronics and Telecommunications Research Institute

15:00 – 15:30 *Self Assembled Monolayers Organized Between Two Metal Surfaces. Correlation Between Electrical Properties and Molecular Structure*
Maria Rampi
University of Ferrara

15:30 – 16:00 *Metal Molecule Semiconductor Device Structures*
Adina Scott
Purdue University

16:00 – 16:30 *Single Electron Transistor Behavior of Self-Assembled Organic Multilayer in Nanogap Electrode*
Takao Ishida
National Institute of Advanced Industrial Science and Technology

16:30 – 16:45 Wrap up and Departure

Poster Presentations

1. **SIMULATION OF BASIC LOGIC GATES USING ASYMMETRICAL MOLECULAR DEVICE MODELS**
   Paul D. Franzon, North Carolina State University

2. **HEATING AND INELASTIC CURRENT IN MOLECULAR STRUCTURES**
   Yu-Chang Chen, University of California, San Diego

3. **MAGNETICALLY DIRECTED SELF-ASSEMBLY OF MOLECULAR MICROSPHERE JUNCTIONS**
   David P. Long, Geo-Centers Inc.

4. **SPECTROSCOPIC CHARACTERIZATION OF MOLECULE-EVAPORATED METAL INTERFACES USING BACKSIDE FTIR AND METAL-MOLECULE-SILICON SAMPLES**
   Christina A. Hacker, National Institute of Standards and Technology

5. **OLIGOMER LENGTH DEPENDENT STUDY OF METAL-MOLECULE INTERACTIONS IN MODEL MOLECULAR WIRE SYSTEMS**
   Chris Zangmeister, National Institute of Standards and Technology

6. **ELECTRONIC TRANSPORT THROUGH SELF ASSEMBLED THIOL MOLECULES: EFFECT OF MONOLAYER ORDER, DYNAMICS AND TEMPERATURE.**
   Geetha R. Dholakia, NASA Ames Research Center

7. **THE ELECTRONIC SPECTRA OF OLIGO(PHENYLENE ETHYNYLENE)'S: AN AB INITIO STUDY OF DIPHENYLACETYLENE**
   Yamil Simón-Manso, Northwestern University and National Institute of Standards and Technology

8. **INVESTIGATION OF TWO STATE CONDUCTANCE SWITCHING IN METAL-MOLECULE-METAL DEVICES BY INELASTIC ELECTRON TUNNELING SPECTROSCOPY**
   Jason L. Lazorcik, Geo-Centers, Inc.

9. **POSSIBLE APPLICATIONS OF CMOL CIRCUITS**
   Konstantin K. Likharev, Stony Brook University

10. **SELF-ASSEMBLY AND TRANSPORT PROPERTIES OF MOLECULES AS SINGLE-ELECTRON TRANSISTORS**
    Konstantin K. Likharev, Stony Brook University

11. **THEORY OF TRANSPORT IN MOLECULAR SINGLE-ELECTRON TRANSISTORS**
    Konstantin K. Likharev, Stony Brook University

12. INVESTIGATION OF CONFORMATIONAL GATING OF ELECTRONIC COUPLING WITHIN A DONOR-BRIDGE-ACCEPTOR SYSTEM VIA OPTICAL MAGNETIC RESONANCE
Emily Weiss, Northwestern University

13. ATOMICALLY PRECISE FABRICATION AND CHARACTERIZATION OF HETEROMOLECULAR ORGANOSILICON NANOSTRUCTURES: IMPLICATIONS FOR SILICON-BASED MOLECULAR ELECTRONICS
Rajiv Basu, Northwestern University

14. OUTER-SPHERE REORGANIZATION ENERGY AS A PROBE OF LIGAND RECEPTOR INTERACTIONS
Matthew R. Hartings, Northwestern University

15. CORRELATED ELECTRONS IN MOLECULAR CONDUCTION
Zsolt Bihary, Northwestern University

16. RIGID MOLECULAR WIRES FROM 1,3- AND 1,4-DISILA/GERMA/STANNABICYCLO[K.L.M]ALKANE MONOMERS (K, L, M = 1 OR 2): INTERESTING SYNTHETICAL TARGETS FOR MOLECULAR ELECTRONICS.
Niclas Sandstrom, Uppsala University

17. FIELD EMISSION CHARACTERISTICS OF A SINGLE FREE STANDING CARBON NANOTUBE WITH GATE ELECTRODE
S. C. Tseng, National Tsing Hua University

18. CHARGE TRANSPORT THROUGH POLY-AROMATIC COMPOUNDS
Revital Cohen, Northwestern Universtiy

19. CHEMICALLY MODIFIED URIDINE FOR USE IN DNA TILES
Wyetta Palmby, University of Notre Dame

20. REVERSIBLE MOLECULAR SWITCHING AT A NANOSCALE METAL-MOLECULAR JUNCTION
Lintao Cai, The Pennsylvania State University

21. ELECTRICAL CHARACTERIZATION OF OPE-BASED MONOLAYERS IN NANOWIRE JUNCTIONS
Marco A. Cabassi, The Pennsylvania State University

22. TRANSPORT CALCULATIONS FOR SINGLE MOLECULES: THEORY AND APPLICATIONS
F. Evers, Research Center Karlsruhe

23. TBA
Tomufumi Tada, The University of Tokyo

24. ELECTRONIC AND TRANSPORT PROPERTIES OF ATOMIC AND MOLECULAR WIRES: THEORETICAL ASPECTS FOR REALIZATION OF SMART NANOSCALE INTERCONNECTS

Rodion Belosludov, Institute for Materials Research, Tohoku University

25. DESIGNS AND SIMULATIONS FOR UNIQUE, COMPACT, SPECIAL-PURPOSE NANOELECTRIC CIRCUITS

James C. Ellenbogen, Nanosystems Group, The MITRE Corporation