Foundations of Nanoscience

Snowbird Cliff Lodge~Snowbird, Utah
April 21- 23, 2004.

Self-Assembled Architectures and Devices

Sponsor: Defense Advanced Research Projects Agency (DARPA)

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The papers in this volume were presented at the Conference "Foundations of Nanoscience: Self-Assembled Architectures and Devices" held in Snowbird, Utah, April 21-23, 2004.

THANKS:
The conference was sponsored by the Defense Advance Research Projects Agency (DARPA). We express our gratitude to Sri Kumar, Program Manager in DARPA / IPTO, for his generous support of this enterprise. Also thanks to Mitra Basu, of the National Science Foundation(NSF) and to K. Birgitta Whaley, Department of Chemistry, University of California, Berkeley, CA, for their aid arranging indirect travel support for some of the invitees via a co-located NSF Workshop on Self-Assembled Architectures. Special thanks also to the Department of Computer Science at Duke University, and in particular to Richard Braun, Courtney Packard, Diane Robinson, Jewel Wheeler for their hours of work on this project.

CONFERENCE OVERVIEW:

The construction of molecular scale structures at the scale of the 1 - 100 nanometer range is one of the key challenges facing science and technology in the twenty-first century. This challenge is at the core of an emerging discipline of Nanoscience, which is at a critical stage of development. There have been some notable successes in the construction of individual molecular components (e.g., carbon nanotubes, and various molecular electronic devices), and the individual manipulation of molecules by probing devices. However, a key deficiency is the lack of methods for constructing complex devices out of large numbers of these molecular components. We need methods to help us hold, shape, and assemble various molecular components into complex machines and systems.

Top-down methods for construction of nanostructures, such as e-beam lithography, have inherent limitations in scale. Bottom-up methods appear to have no such scale limitations. Self-assembly is a bottom-up method of construction where substructures are spontaneously self-ordered into superstructures driven by the selective affinity of the substructures. While top-down methods are well understood, and widely used in engineering and manufacturing processes, self-assembly is a much less well-understood construction process. Chemists have for many decades used self-assembly methods (for example, for the self-assembly of lipid or polymer layers), but they conventionally result in structures with limited complexity, and are not readily programmable. However the cell is self-assembled, and contains many complex structured components.

A missing pillar in the emerging discipline of Nanoscience is an understanding of self-assembly methods for forming complex structured components. For a variety of historical reasons, self-assembly processes and experiments have not been examined by science to the degree that is now needed by Nanoscience. It is intended that the Conference will provide a synergism for a community of scholars working in self-assembly related areas who would otherwise not have contact with each other. In summary, the Conference Foundations of Nanoscience was intended to have a major impact on the emerging field of nanoscience and self-assembly, by getting those people working in self-assembly in the same place for the first time. It is intended that the Conference on Foundations of Nanoscience is to be held annually in subsequent years.

John Reif, March 2004

CONFERENCE ORGANIZATION:

Program Chair: John Reif
Department of Computer Science, Duke University, Durham, NC
Email: reif@cs.duke.edu
Phone: 919-660-6568

Program Committee: Track Chairs

Track on Principles and Theory of Self-Assembly:
Track Chair: Leonard Adleman, Laboratory for Molecular Science, University of Southern California. Los Angeles, CA

Track on Self-Assembled DNA Nanostructures:
Track Chair: Nadrian Seeman, Department of Chemistry, New York University, New York, NY

Track on Self-Assembled Surface Chemistry:
Track Chair: Lloyd Smith, Department of Chemistry, University of Wisconsin, Madison, WI

Track on Peptide and Viral Self-Assembly
Track Chair: Michael Hecht, Department of Chemistry, Princeton University, Princeton, NJ

Track on Conformal, Magnetic & Hydophobic-Hydrophilic Self-Assembly:
Track Chair: Karl Bohringer, Department of Electrical Engineering, University of Washington, Seattle, WA

Track on DNA-Metal Aggregates:
Track Chair: George C. Schatz, Department of Chemistry, Northwestern University, Evanston, IL

Track on Molecular Electronics Devices:
Track Chairs: James R. Heath, Department of Chemistry, California Institute of Technology, Los Angeles, CA & Kwan Kwok, Microsystems Technology Office (MTO), Defense Advanced Research Projects Agency (DARPA), Arlington, VI

Track on Molecular Electronics Architectures:
Track Chairs: R. Stanley Williams & Philip J. Kuekes, Hewlett-Packard Corporation, Palo Alto, CA

Track on Molecular Motors:
Track Chair: Andrew Turberfield, Department of Physics, Oxford University, Oxford, UK

Track on Fullerene Nanostructures:
Track Chair: Jie Liu, Department of Chemistry, Duke University, Durham, NC

Track on Molecular Sensors:
Track Chair: Homme Hellinga, Department of Biochemistry, Duke University Medical School, Durham, NC

Track on New Funding Program Ideas
Track Chair: Sri Kumar, Information Processing Technology Office(IPTO), Defense Advanced Research Projects Agency (DARPA), Arlington, VI

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Track Chair: Leonard Adleman, Laboratory for Molecular Science, University of Southern California. Los Angeles, CA

Track Chair Overview Paper:
- Toward a general theory of Self-assembly
Leonard Adleman

Session A Invited Papers:

- Phase Transitions and Control in Self Assembly
Ed Coffman, Department of Computer Science, Columbia University, NY City, NY

- Self assembling by DNA junction molecules: the theoretical model
Natasha Jonoska, Department of Mathematics, University of Southern Florida, Tampa FL

- Directed Self-Assembly Using Graph Grammars
Eric Klavins, Dept of Electrical Engineering, University of Washington, Seattle, WA

- Flux systems, flows and self-assembly
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Erik Winfree, California Institute of Technology, Pasadena, CA

- Optimal Self-Assembly of Counters at Temperature Two
Ashish Goel, Qi Cheng and Pablo Moisset de Espanes, Department of

Management Science and Engineering, Stanford University, Stanford CA

- Compact Error-Resilient Computational DNA Tiling Assemblies
Sudheer Sahu, Department of Computer Science, Duke University, Durham, NC

FNANO Track on DNA-Metal Aggregates
Track Chair: George C. Schatz, Department of Chemistry, Northwestern University, Evanston IL

Track Chair Overview Paper:
- Cooperative DNA Melting in DNA Linked Gold Nanoparticle Aggregates
George C. Schatz

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Yi Cui and Paul Alivisatos, University of California, Berkeley, CA

- Nanopearls: A new synthesis for programmably creating Biochemical-Nanoparticle linear sequences and applications
Joe Jacobson, Media Lab, MIT, Cambridge, MA and Shuguang Zhang, Center for Biomedical Engineering, MIT, Cambridge, MA

- DNAzyme-Directed Assembly of Nanoparticles and its Application as Colorimetric Sensors for a Broad Range of Analytes
Yi Lu, Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana, IL

- Self-Assembly Driven Metallization of DNA-Templated Nanowires
Oliver Harnack, Materials Science Laboratories, Sony International (Europe) GmbH, Stuttgart, Germany

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- DNA-based fabrication of metallic wires and networks
Michael Mertig, Institut für Werkstoffwissenschaft, Technische Universität Dresden, Dresden, Germany

- Polymer-Gold Aggregates
Sungho Park, Department of Chemistry, Northwestern University, Evanston IL

- Transistor in a Test Tube - Harnessing Molecular Biology to the Self-Assembly of Functional Electronics
Uri Sivan, Department of Physics, Technion, Haifa, Israel

FNANO Track on Molecular Electronic & Quantum Devices
Track coChairs:
James R. Heath, California Institute of Technology, Los Angeles, CA and
Kwan Kwok, Microsystems Technology Office (MTO), Defense Advanced Research Projects Agency (DARPA), Arlington, VI

Track Chair Overview Paper:
Molecular Mechanics & Electronics
James R. Heath

Session A Invited Papers:

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Hongjie Dai, Department of Chemistry, Stanford University, Stanford, CA

- STM spectroscopy on free-standing carbon nanotubes
Cees Dekker, Delft University of Technology, Department of Applied Physics, The Netherlands

- Four Unimolecular Rectifiers and What Lies Ahead
R. Metzger, Chemistry Department, University of Alabama, Tuscaloosa, AL

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- Polymeric Nanofibers and Nanowire Devices
David Bocian, University of California at Riverside, Riverside, CA

- Polymer Nanofiber Based Devices
Harold G. Craighead, Cornell University, Ithaca, NY

- Building Block Approaches to Molecular Nanomagnets

Kim Dunbar, Dept. of Chemistry, Texas A&M University, College Station, TX

- Silicon contacts: A new playground for molecular electronics?
Avik Ghosh, School of Electrical and Computer Engineering, Purdue University, West Lafayette, IN

- Self-Assembly and Lithographic Patterning of DNA Rafts
Marya Lieberman, Department of Chemistry and Biochemistry, University of Notre Dame, Notre Dame, IN

- In-wire Molecular Electronic Devices: Synthesis and Electrical Characterization
Theresa Mayer, Pennsylvania State University, University Park, PA

- Molecular Mechanics & Electronics
Fraser Stoddart, UCLA & California NanoSystems Institute(CNSI), Los Angeles, CA

- Synthesis and Self-Assembly of Nanostructures
Younan Xia, Department of Chemistry, University of Washington, Seattle, WA

- Design of Magnetic Spinel Ferrite Nanoparticles for Biological Applications
John Zhang, School of Chemistry & Biochemistry, Georgia Institute of Technology, Atlanta, GA

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- Carbon Nanotube Electronics and Opto-electronics
Phaedon Avouris, Nanometer Scale Science & Technology, IBM Research Division, T.J. Watson Research Center, Yorktown Heights, NY

- Some Issues of Junction Dynamics
Mark Ratner, Chemistry Department, Northwestern University, Evanston Il

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Mark Reed, Department of Electrical Engineering, Yale University, New Haven, CT

- Molecular Electronics: NanoCell Electronic Memories and Direct Covalent Attachment of Molecules to Oxide-Free Silicon for Construction of Hybrid Devices
James Tour, Department of Chemistry, Rice University, Houston, TX

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David Awschalom, Department of Physics, University of California, Santa Barbara, CA

- Molecular Quantum-dot Cellular Automata
Craig Lent, Department of Electrical Engineering, University of Notre Dame, Notre Dame, IN

- Quantum Computation with Endohedral Fullerenes
Jason Twamley, Department of Mathematical Physics, National University of Ireland Maynooth, Kildare, Ireland

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FNANO Track on Peptide and Viral Self-Assembly

Track Chair: Michael Hecht, Department of Chemistry, Princeton University, Princeton, NJ

Track Chair Overview Paper:
- Structures and Functions of De Novo Proteins from Designed Combinatorial Libraries
Michael Hecht

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- Virus-Based Genetic Toolkit for the Directed Synthesis of Magnetic and Semiconducting Nanowires
Angela Belcher, MIT, Cambridge, MA

- Chemical and Genetic Tailoring of Virus Particles to Achieve Nanochemical Function
M.G Finn, Department of Chemistry and The Skaggs Institute for Chemical

Biology, Scripps Research Institute, La Jolla, CA

- Self-Assembled Viruses as Nanocontainers
William Gelbart, Department of Chemistry, UCLA, Los Angeles, CA

-Assembly and Functionization of an Icosahedral Virus
Tianwei Lin, Scripps Institute, La Jolla, CA -Tianwei Lin <twlin@scripps.edu>, Scripps Institute, La Jolla, CA

- Peptide and Biomimetic Catalysts for Structure-Directed Nanofabrication of Siloxanes, Organometallics and Metallo-oxanes
Daniel Morse, Department of Molecular, Cellular and Developmental Biology, UC Santa Barbara, Santa Barbara, CA

- Molecular Biometics: Building Materials via the Natures's Way, One Molecule at a Time
Mehmet Sarikaya, University of Washington, Seattle, WA

FNANO Track on Molecular Motors

Track Chair: Andrew Turberfield, Department of Physics, Oxford University, Oxford UK

Track Chair Overview Paper:
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Andrew Turberfield

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Alberto Credi, Department of Chemistry, University of Bologna, Italy

- Artificial Surface-Mounted Molecular Rotors
Josef Michl, Department of Chemistry and Biochemistry, University of Colorado, Boulder, CO

- DNA Nanoactuator in Self-assembly
Hao Yan, Department of Computer Science, Duke University, Durham, NC

- Autonomous DNA Motors and Computing Machines: Experimental Study

and Theoretical Constructions
Peng Yin, Department of Computer Science, Duke University, Durham, NC

Session B Invited Papers:

- Nanodevices integrating biomolecular motors
Henry Hess, Department of Bioengineering, University of Washington, Seattle, WA

- Construction of micro belt conveyers: two approaches
Taro Uyeda, Gene Function Research Center, Tsukuba Central, Ibaraki, Japan

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FNANO Track on Molecular Sensors
Track Chair: Homme Hellinga, Department of Biochemistry, Duke University, Durham, NC

Track Chair Overview Papers:
- Computational design of protein-based biosensors
Homme Hellinga

Invited Papers:

- Massive Self-Assembly of Carbon Nanotube-Based Integrated Sensor Structures
Seunghun Hong, Department of Physics, Florida State University

- Nanodevices based on linear protein molecular motors: Challenges and opportunities
Dan Nicolau, Swinburne Industrial Research Institute, Swinburne University of Technology, Swinburne, Australia

- S-layers as patterning elements for supramolecular structures
Dietmar Pum and Uwe Bernd Sleytr, Center for Ultrastructure Research, University of Natural Resources and Applied Life Sciences, Gregor Mendel-Strasse 33, A-1180 Wien, Austria

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FNANO Track on Conformal, Magnetic, Electrostatic & Hydophobic-Hydrophilic Self-Assembly

Track Chair: Karl Bohringer, Department of Electrical Engineering, University of Washington, Seattle, WA

Track Chair Overview Paper:
Programmable Surfaces: Toward Massively Parallel Self-Assembly at the Micro- and Nano-scale
Karl Bohringer

Invited Papers:

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- Magnetic Self-Assembly "Equilibria" at a Macroscopic Scale
Geoge C. Lisensky, University of Wisconsin, Madison, WI

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John Stephen Smith, Dept EECS, University California Berkeley, Berkeley, CA

FNANO Track on Self-Assembled Surface Chemistry
Track Chair: Lloyd Smith, Department of Chemistry, University of Wisconsin, Madison, WI

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Lloyd Smith, Department of Chemistry, University of Wisconsin, Madison, WI

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David Allara, Pennsylvania State University, University Park, PA

- Oriented Immobilization of Single DNA Molecules as a Tool for Surface Structuring on the Nanometer Scale
Frank F. Bier, Fraunhofer Institute for Biomedical Engineering and University of Potsdam, Bergholz-Rehbruecke, Germany

- Patterning Self-assembled monolayers using a scanning probe: Technique and Utility
Christopher Gorman, Department of Chemistry, North Carolina State University, Raleigh, NC

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Francesco Stellacci, Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA

- Creating Nanostructures through Self- and Directed Assembly
Paul Weiss, Pennsylvania State University, University Park, PA

FNANO Track on Molecular Electronics Architectures

Track coChairs:
Philip J. Kuekes, Hewlett-Packard Corporation, Palo Alto, CA and
R. Stanley Williams, Hewlett-Packard Corporation, Palo Alto, CA

Track Chairs' Overview Paper:
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Philip J. Kuekes and R. Stanley Williams

Invited Papers:

- System Architectures & System Simulations for Molecular Electronic Nanomemories and Nanoprocessors
James Ellenbogen, MITRE Corporation, McLean VA

- Integration for Molecular Electronics
Paul Franzon, Department of Electrical and Computer Engineering, North

Carolina State University, Raleigh, NC

- Circuit and System Architecture for DNA-Guided Self-Assembly of Nanoelectronics
Alvin Lebeck, Department of Computer Science, Duke University, Durham, NC

FNANO Track on Fullerene Nanostructures

Track Chair: Jie Liu, Department of Chemistry, Duke University, Durham, NC

Track Chair Overview Paper:
Direct Growth of Long and Aligned Single Walled Carbon Nanotubes for Nanoscale Electronic Applications
Jie Liu

Invited Papers:

- Simulations of nanotube-based structures and devices
Jerry Bernholc, Department of Physics, North Carolina State University(NCSU), Raleigh, NC

-Fundamental Properties and Applications of Semiconducting Carbon Nanotubes
Michael Fuhrer, Department of Physics, University of Maryland, College Park, MD

- Growth of SWNT with controlled structure by tailoring catalyst composition and reaction environment
Daniel E. Resasco, School of Chemical Engineering and Materials Science, University of Oklahoma, Norman, OK

- Designing Carbon-Based Nanotechnology on a Supercomputer
David Tomanek, Department of Physics and Astronomy, Michigan State University, East Lansing, MI

- Controlled assembly of carbon nanotube structures and devices
Otto Zhou, Material Science, Department of Physics, University of North

Carolina (UNC), Chapel Hill, NC

Poster Abstracts:

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Yuliy Baryshnikov, Bell Labs, Lucent Technologies, Murray Hill, NJ

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Chris Dwyer, Department of Computer Science, Duke University, Durham, NC

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Alberto Di Fabio, Department of Chemistry, University of Bologna, Bologna, Italy

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Vijeta Johri, Department of Computer Science, Duke University, Durham, NC

Active and Dynamic Nanomaterials Using Kinesin and Microtubules
Steven John Koch, Biomolecular Materials and Interfaces, Sandia National Laboratories, Albuquerque, NM

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Robert M. Dirks, Milo Lin, Erik Winfree, and Niles A. Pierce, Applied & Computational Mathematics, California Institute of Technology, Pasadena, CA

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Sung Ha Park, Department of Physics, Duke University, Durham, NC

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Jaidev Patwardhan, Department of Computer Science, Duke University, Durham, NC

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K. Birgitta Whaley, Joshua Schrier and Laxmidhar Senapati, Department of Chemistry, University of California, Berkeley, CA