

Synergy Between Experiment and Computation in Nanoscale Science

May 31 to June 3, 2006
Harvard University, Cambridge, MA

Conference Schedule

Tuesday, May 30

7:30 Welcome Reception
Informal reception at the Sheraton Commander Hotel
lobby and in the Café-lounge. Badges available here.

Day One (all talks in Maxwell-Dworkin G115)
Wednesday, May 31

8:00 Breakfast and registration
Maxwell-Dworkin ground floor lobby

8:55 **Sandip Tiwari**, NNIN Director
Welcome Address

9:00 **Venkatesh Narayanamurti**, Dean of the Division of Applied Sciences and
Engineering at Harvard University
Opening Address

CASIMIR EFFECT

9:10 I **Federico Capasso** (invited), Harvard University

9:50 II **Steven Johnson** (invited), Massachusetts Institute of Technology

10:20 III **Hideaki Taniyama**, NTT, Japan
*Radiation Force in High-Q Double-Layer Cavities of Two-Dimensional
Photonic Crystal Slabs*

10:40 IV **René Sedmik**, ARC Seibersdorf, Austria
*Detailed Parametric Study of Casimir Forces in the Casimir Polder
Approximation for Nontrivial 3D Geometries*

11:00-11:30 Break

GENERAL PHOTONICS

11:30 I **John Joannopoulos** (invited), Massachusetts Institute of Technology

12:10 II **Edward Sargent**, University of Toronto, Canada
Fast and Accurate Design of Photonic Crystal Devices

12:30-2:00 Lunch
Maxwell-Dworkin ground floor lobby

GENERAL PHOTONICS (continued)

2:00 III **Teri Odom**, Northwestern University
Manipulation of Light in Anisotropic Nanostructures: Hole Arrays and Pyramids

2:20 IV **Michelle Povinelli**, Stanford University
Slowing and Stopping Light in Photonic Crystals: Theory and Experiments

2:40 V **Dario Gerace**, ETH Zurich, Austria
Cavity-QED with photonic crystal nanocavities and semiconductor quantum dots

3:00 VI **Nader Engheta**, University of Pennsylvania
Lumped Nanocircuit Elements and Circuit Theory in Nanooptics-- Optical-Field Nanoelectronics

3:20-3:40 Break

NANO TRANSPORT: ATOMS AND WIRES

3:40 I **Latha Venkataraman**, Columbia University
Well-Defined Single Molecule Circuits: Why do Amine-Gold Linkages Work? Part I

4:00 II **Mark Hybertsen**, Columbia University
Well-Defined Single Molecule Circuits: Why do Amine-Gold Linkages Work? Part II

4:20 III **Bhaskaran Muralidharan**, Purdue University
Quantitative theories for single molecule conduction: Formal and computational challenges

4:40 IV **Morten Stilling**, Nano-Science Center, Denmark
Electronic Transport in Crystalline Magnetotunnel Junctions: Effects of Structural Disorder

5:00 V **Bart Partoens**, University of Antwerp, Belgium

Structural and electronic properties of B- and P-doped silicon nanowires: first-principles calculations

7:30 -10:30 Computer Session
Science Center Basement

Day Two
Thursday, June 1

8:00 Breakfast
Maxwell-Dworkin ground floor lobby

2DEG TRANSPORT

9:00 I **David Goldhaber-Gordon** (invited), Stanford University
Understanding how electrons organize themselves in tight quarters

9:40 II **John Shumway** (invited), Arizona State University

10:20-10:50 Break

2DEG TRANSPORT (continued)

10:50 III **Eric Heller** (invited), Harvard University
Imaging electron flow in 2DEGS with and without a magnetic field

11:10 IV **Arindam Ghosh**, University of Cambridge, United Kingdom
Experimental Observation of 2D Kondo Lattice in Nonmagnetic Semiconductor Heterostructures

11:30 V **Sheena Murphy**, University of Oklahoma
Spin Focusing in InSb Heterostructures

11:50 VI **Svetlana Anissimova**, Northeastern University
Comparison between experiment and Punnoose-Finkelstein theory of the metal-insulator transition in 2D electron systems

12:10 VII **Michael Fogler**, University of California, San Diego
Scanned gate microscopy of a one-dimensional quantum dot

12: 30-2:00 Lunch
Maxwell-Dworkin ground floor lobby

MICROFLUIDICS

2:00 I **Howard Stone** (invited), Harvard University

The interplay between computation and experiments for new understanding and device development in microfluidics

2:40 II **Luca Biferale**, University of Rome, Italy
Dewetting transitions on micro-corrugated surfaces: a mesoscopic approach

3:00 III **Boris Khusid**, New Jersey Institute of Technology
Electric field driven transport phenomena at nanoscale

3:20 IV **Metin Muradoglu**, Koç University, Turkey
Computational Modeling of Interfacial Flows in Microchannels

3:40-4:00 Break

MICROFLUIDICS (continued)

4:00 V **Sauro Succi** (invited), Istituto per le Applicazioni del Calcolo, Italy
A Lattice Boltzmann-Molecular Dynamics multiscale approach to the numerical simulation of DNA translocation

4:40 VI **Thomas Ward**, University of California, Los Angeles
Squeezing and de-wetting of a drop between plane parallel surfaces: a model problem for understanding capillary adhesion phenomenon

5:00 VII **Manju Prakash**, Cornell University
Mechanism of Heat transfer in Nanofluids

5:20 VIII **Jacob Eapen**, Massachusetts Institute of Technology
The Role of Potential Energy Fluctuations in the Thermal Transport of Nano-colloids

6:00-8:00 Poster Session
Maxwell-Dworkin ground floor lobby

Day Three
Friday, June 2

8:00 Breakfast
Maxwell-Dworkin ground floor lobby

CORRELATION AND DOTS

9:00 I **Charles Marcus** (invited), Harvard University

9:40 II **David Guy Austing**, National Research Council, Canada
Probing by transport the single-particle energy spectrum up to high energy of one quantum dot with the ground state of an adjacent weakly coupled

quantum dot: A way to probe how circular and parabolic vertical quantum dot confinement potential can be

10:00 III **Mark Gyure**, HRL Laboratories
Synergy between Experiment and Computation in Developing and Characterizing Vertical "Enhancement Mode" Quantum Dot Devices

10:20 IV **Guy Ramon**, University at Buffalo, SUNY
Dynamic nuclear spin polarization in gated double quantum dots

10:40 V **Lev Mourokh**, Queens College, CUNY
Fano resonances in the system of coupled quantum point contacts

11:00-11:30 Break

AB INITIO

11:30 I **Normand Modine** (invited), Sandia National Laboratories
Nano is Big: A First-Principles Electronic Structure Viewpoint

12:10 II **Rajesh Sathiyarayanan**, University of Maryland
Multi-site Interactions--Implications and Sensitivity to Relaxation of Adatoms: Density Functional Theory Calculations

12:30-2:00 Lunch
Maxwell-Dworkin ground floor lobby

NANOSTRUCTURES

2:00 I **Derek Stewart** (invited), Cornell University
Nanotube Optoelectronics: Detecting light in the nanoscale world

2:40 II **Gerhard Klimeck** (invited), Purdue University

3:20 III **Vasili Perebeinos**, IBM
Transport and Optical Properties of Carbon Nanotubes

3:40-4:00 Break

NANOSTRUCTURES (continued)

4:00 IV **Cheol-Hwan Park**, University of California, Berkeley
Excitonic Effects and Optical Spectra of Single-Walled Boron Nitride Nanotubes

4:20 V **Fotios Papadimitrakopoulos**, University of Connecticut
Diameter and Metallicity Fractionation and Modeling of Single Wall Carbon Nanotubes according to Redox Differences

- 4:40 VI **Ralph Nuzzo**, University of Illinois, Urbana-Champaign
The Strange Non-Bulk Properties of Nanoscale Materials: Negative Thermal Expansion of γ -Alumina-Supported Pt Catalysts
- 5:00 VII **Mina Yoon**, Oak Ridge National Laboratory
The Role of Defects in Determining the Structural Stability of Carbon-based Nanomaterials
- 5:20 VIII **Chenggang Tao**, University of Maryland
Ag islands decorated by C₆₀
- 7:00-9:00 Conference Banquet
Maxwell-Dworkin ground floor lobby

Day Four
Saturday, June 3

- 8:00 Breakfast
Maxwell-Dworkin ground floor lobby

NANO BIO

- 9:00 I **George Whitesides** (invited), Harvard University
Comments and Suggestions for Problems at the Interface between Computation/Simulation and Materials Science
- 9:40 II **Robert Johnson**, University of Pennsylvania
Molecular Dynamics Simulations of DNA Functionalized Carbon Nanotube Chemical Sensors
- 10:00 III **Vittorio Cristini**, University of California, Irvine
Virtual Cancer: Towards the Development of Integrated Computational and Experimental Models
- 10:20 IV **Brian Pereira**, Rensselaer Polytechnic Institute
Autocatalytic Reactions of Inteins: Insights from Molecular Dynamics, Quantum Mechanics, and Molecular Biology
- 10:40 V **Cengiz Özkan**, University of California, Riverside
Carbon Nanotube-DNA Nanoarchitectures and Electronic Functionality
- 11:00-11:20 Break
- 11:20 **Sadasivan Shankar** (invited), Intel Corporation
- 12:00-2:00 Grace Notes

Extended lunch, with string quartet, for collaboration and networking; outdoors (weather permitting) near Maxwell-Dworkin entrance. (otherwise in Maxwell-Dworkin ground floor lobby).