DMR Perspective

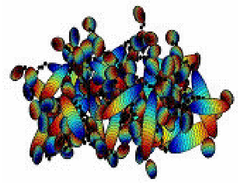
W. Lance Haworth, Acting Director, DMR
Solid State Sciences Committee Meeting
NAS, Washington, DC
19 April 2007

Outline

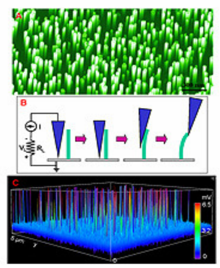
- Status, outlook & challenges for DMR & CMMP
- Computational physics
- Future of electronics
- Specific examples
  - for your reading enjoyment

We seek a fundamental understanding of materials and condensed matter

Can we create new materials for science and technology?



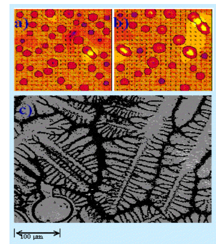
Can we understand and apply the physics of condensed matter?



How can we understand and exploit the nano-world?

"TRANSFORMATIVE MATERIALS"

Can we understand and control processing/structure/properties relationships in engineering materials?



How can we explore and develop the frontier between materials and biology?

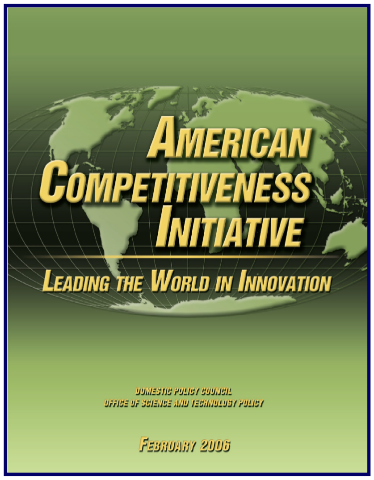
Division of Materials Research

Focus for Diverse Communities and Funding Modes

NSF support for materials research is not limited to DMR

- *Programs for Individual Investigators and Groups*
  - **Condensed Matter and Materials Theory, Condensed Matter Physics**
  - **Solid State Chemistry, Polymers, Biomaterials**
  - **Metals, Ceramics, Electronic/Optical Materials**
- *Cross-cutting Programs*
  - **Centers, Institutes & Partnerships**
  - **User Facilities and Instrumentation**
  - **Office of Special Programs (International Collaboration; Education)**
- *Distributed Mechanisms*
  - **Focused Research Groups**
  - **NSF-wide programs – *REU/RET, CAREER, GOALI, MRI, etc***
  - ***DMR is a major partner in NSF-NANO***
- *Connections*
  - **Other areas of NSF, other federal agencies, international, industry**

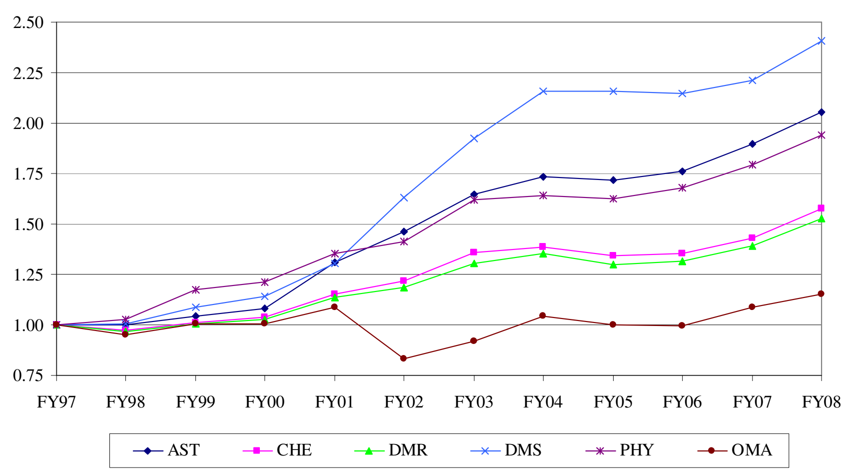
Everything DMR supports is relevant to American competitiveness!



- Emphases
  - Tie fundamental discoveries to marketable technologies
  - Facilities and instrumentation
  - World class science and engineering workforce
  - Focus on Phys Sci & Engineering
- Doubles NSF, DOE-OS, NIST over 10 years
- Biggest federal response since Sputnik

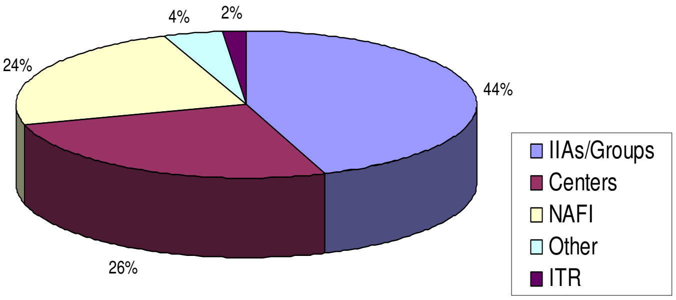
Directorate for Mathematical & Physical Sciences

Funding History, 1997-2008*



DMR Program Balance

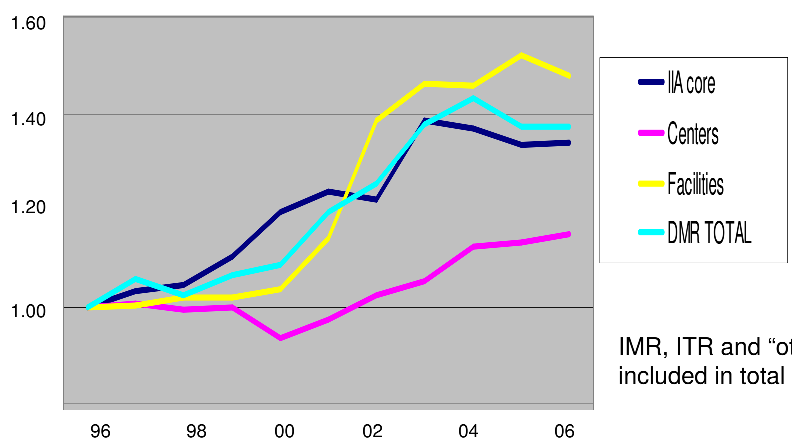
FY 2006
$252.2M
(includes MRI)



"About right – but don't erode support for individuals and small groups" - COV

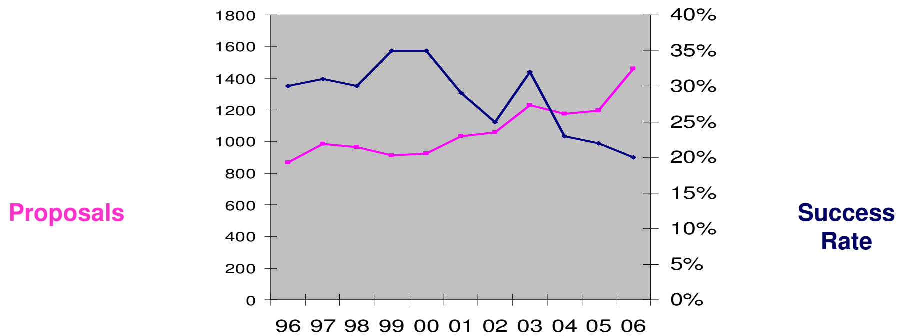
DMR Funding History, 1996-2006

$242.6M in FY06



IMR, ITR and "other" included in total

DMR Proposal Pressure & Success Rates (Research Grants)



- Many strong proposals declined essentially for lack of funds
- Grant sizes not keeping pace with 'scientific' inflation
- Success rates vary but NSF-wide average is no better

MPS by Division

	FY 2005 Actuals	FY 2006 Actuals	Change from 05 to 06	FY 2007 Request	Change from 06 to 07	FY 2008 Request	Change from 07 to 08
AST	195.11	$199.75	2.4%	$215.11	7.7%	$232.97	8.3%
CHE	179.26	180.70	0.8%	191.10	5.8%	210.54	10.2%
DMR	240.09	242.59	1.0%	257.45	6.1%	282.59	9.8%
DMS	200.24	199.52	-0.4%	205.74	3.1%	223.47	8.6%
PHY	224.86	234.15	4.1%	248.50	6.1%	269.06	8.3%
OMA	29.80	29.9	0.3%	32.40	8.4%	34.37	6.1%
Total, MPS	1,069.36	1,086.61	1.6%	1,150.30	5.9%	1253.00	8.9%
R&RA	4234.82	4449.25	5.1%	4,765.95	7.1%	5,131.69	7.7%
NSF	5480.78	5645.79	3.0%	6,020.21	6.6%	6429.00	6.8%

Management Challenges

- Success rates and grant sizes
- Broadening participation
- Support for young faculty
- Balance among funding modes
- "Transformative" research
- Instrumentation and facilities
  - ***Bench-scale, mid-scale, and large scale / stewardship***
  - ***Light source panel***
- Collaborative research on complex problems
  - ***Centers, groups, networks***
  - ***Cooperation: across NSF, interagency, international***
- *ACI is our huge opportunity*

Broadening Participation

"The Under-represented **Majority**" – *Shirley Jackson*

DMR Competitive Awards to Women and Minorities

Women

(66/375 in FY06)

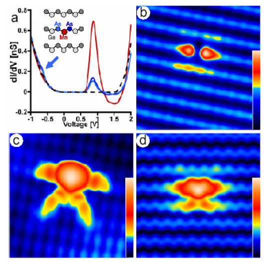
Minority

(34/375 in FY06)

- **Gender Equity & BP Workshops – Chemistry, Physics, MS&E**
- **Partnerships for Research and Education in Materials (PREMs)**
- **Division reserve co-funding**

Intellectual Challenges
FY 08 DMR Focus Areas

- ***Via 'core' programs wherever possible***
- Nanoscale materials and phenomena
- Computational discovery and innovation
- Complex systems including *biomaterials*
- Fundamental research addressing "Science Beyond Moore's Law"
- ***Expect the unexpected!***



Education is integrated throughout

Computational Physics

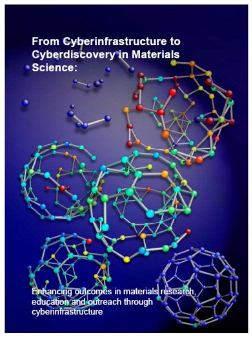
- Computational physicists working with experimentalists
  - ***Thin Layer Flow*** - Michael Shearer, Karen Daniels (NCSU) - new
  - ***Statistical Mechanics of Turbulence*** - Gustavo Gioia, Nigel Goldenfield, Walter Goldburg (UIUC, Pitt) - new
- Materials by design
  - ***Combining data mining + QM*** – Gerbrand Ceder & Dane Morgan
- Real time analysis of experiments
  - ***DANSE - neutron scattering analysis*** – Brent Fultz, CalTech / SNS
- Computation and future electronics overlap
  - ***Institute for Theory of Advanced Materials in IT*** – Jim Chelikowsky et al
  - ***QM simulation of electron storage device*** - Nicola Spaldin
  - ***Quantum Interference Transistor –*** Charles Stafford et al
- Complexity – connecting across length & time scales
  - ***Mechanical response of nanocrystal*** - Izabel Szlufarska et al

Cyber-enabled Discovery and Innovation

It's a 2-way street:

Materials enable CI

CI will change the way we do research



Simon Billinge, Michigan St

Ernest Fuentes, Cornell/CHESS

Mark Novotny, Mississippi St

Krishna Rajan, Iowa St

Bruce Robinson, U Washington

Fred Sachs, SUNY-Buffalo

Susan Sinnott, U Florida

Horst Henning Winter, U Mass

Read the report, see presentations and post comments at
www.mcc.uiuc.edu/nsf/ciw_2006/

CI / Materials Workshop Summary

Impact of materials research on CI

- Materials science research … is the enabling technology underpinning all of CI developments
- Evolutionary and revolutionary developments in CI will be closely coupled to breakthroughs in basic materials research
- DMR has a unique role and responsibility
- Historical importance of 'blue sky' and fundamental research
- Importance of funding tools and methodologies that underpin this research, especially in nanosciences
- A number of research frontiers may result in CI revolution
  - ***not clear which will succeed***
  - ***fund as broadly as possible***

CI / Materials Workshop Summary

Impact of CI on materials research

- Enormous potential for creative application of CI tools
- Greatest impacts likely to be unexpected ones
- Aspects of materials research that will clearly benefit from CI investment:
  - ***Materials theory remains at cutting edge***
  - ***Investment in user facilities not yet matched by software and CI investments to exploit them***
  - ***Broaden access and enhance educational benefits for facilities***
  - ***Special role in building community***
  - ***Software developments will lead to new / better / more science***
  - ***Algorithm development will always lead to breakthroughs***
  - ***Full exploitation of materials databases; creation and curation of high quality databases; (cf. bio)***
- Critical issues

CMMT - A Few Intellectual Challenges

"Challenges of many interacting particles"

- Discover new classes of matter, emergent properties and phenomena, and ways to control them
- From the fundamentals, predict the structure and properties of matter and materials
- Non-equilibrium statistical mechanics: from fracture to life
- Interconnecting seemingly diverse phenomena: the synergy of research across disciplines

Courtesy of CMMT program directors

Future of Electronics
Materials Challenges & Issues

Courtesy of EM program directors

- **Understanding fundamental chemical and physical interface phenomena and properties**
  - **Thin film properties** differ significantly from bulk materials, can critically depend on, and be tailored by surface/interface phenomena
  - **Greater integration of dissimilar materials** is essential for advanced electronics, and for combined electronic and photonic functionalities.
- **Heteroepitaxy remains a challenging subject of vital importance in growth of thin films, superlattices, and quantum dots for electronics/photonics**
- **Organic electronic/photonic materials**
  - **Organic materials** offer lower cost, mechanical flexibility, and a range of performance to provide cost/performance advantages, for some significant electronic/photonic applications including displays, lighting, solar energy conversion, and high speed optical modulation.
  - Major challenges include identification and synthesis of suitable materials with **required properties and long lifetime**. In the case of solar energy conversion, for example, increasing energy conversion efficiency continues to be a major challenge.

Future of Electronics
Materials Challenges & Issues

Courtesy of EM program directors

BEYOND CMOS:

- Research on **fundamental aspects of materials design, synthesis, processing** needed to support new paradigms in electronics beyond CMOS.
- Such structures may include **molecular electronics, spin FETs (field-effect transistors), single electron transistors, nanotube FETs, and nanowire transistors.**

- **Molecular electronics**
  - **NSF Workshop**, June 7-8, 2007 (CHE/DMR/ENG): To identify where and how molecules can be used in electronic systems and delineate the scientific and technical challenges to realizing that vision
- **Spin electronics**
  - **Coherent spins** providing information in phase; low power; increased speed
  - **Coupled single spins** providing information in entanglement; new paradigm for computation and communication ***(Newcomb-Cleveland prize 2006)***
- **Nanostructured materials**
  - Active positioning of single dots within photonic cavities is important for exploring **coupled Cavity-Quantum Electrodynamic phenomena** which may lead to unique single photon sources and/or entangled photon pair generation.
  - **Quantum dot arrays** fabricated with low dispersion in size and spacing are of interest for electronics/photonics, but have been elusive.

Future of Electronics

- Science "Beyond Moore's Law"
  - ***Hardware, Architecture, Algorithms, Software***
  - ***Long-term alternatives to CMOS?***
- *New materials, new physics, and more surprises*
  - ***Graphene*** – *relativistic electron transport* (Fertig); QHE @ RT
  - ***Superconductivity in a ferromagnetic 'half-metal'*** (Alabama MRSEC)
  - ***Quantum effects in single-molecule magnets*** (Andrew Kent et al)
- Spin electronics
  - Dave Awschalom & Nitin Samarth; Ali Yazdani; Jagadeesh Moodera; Giti Khodaparast; S-C Zhang; Alan MacDonald; Giovanni Vignale; Joel Moore…
- Nano-realm, surfaces, wires, interconnects, addressability
  - ***Quantum properties of nanostructures*** (A.Bezryadin; Nadya Mason)
  - ***Ohm's Law in Smart Materials*** (Freericks, Liu, Jones)
  - ***Electron-phonon coupling at semiconductor surfaces*** (Himpsel)
  - ***Semiconductor nanomembranes*** (Lagally et al., Wisconsin MRSEC)

Future of Electronics

- Molecular electronics

  Patterning large organic semiconductor arrays
  - Fred Wudl, Zhenan Bao et al., Stanford MRSEC

  A molecular transistor
  - Andrew Kent; Dan Ralph; Charles Stafford & Sumit Mazumdar

  Metal-organic bonds; metal-nanotube contacts
  - Ellen Williams et al, U Md MRSEC
  - Cha, Muller, Briere, Arias, Cornell MRSEC

  Invisible optoelectronics
  - *Tobin Marks et al,* NWU MRSEC
- Quantum computation

  Can we employ electrons in new ways to make devices?
  - Chetan Nayak, M. Freedman, Sankar Das Sarma

  Do we need electrons for 'electronics'?
  - David DeMille, Robert Schoelkopf, Steve Girvin

Current & future growth areas for CMMP

- New quantum states of matter
- Interface with AMOP
- Quantum-classical interface, including nano
- Interface of ‘soft’ and ‘hard’
- Interface with bio
- New architectures for quantum computing
- Emergent behavior & complexity
- Computation in real time during experimentation

Courtesy of CMP program directors

Emergent Phenomena in Condensed Matter

“A traditional route to understanding these kinds of emergent states is to create them in new materials. In this way, one can study states with different characteristics and either test theoretical descriptions of such states or realize entirely new states of matter.”

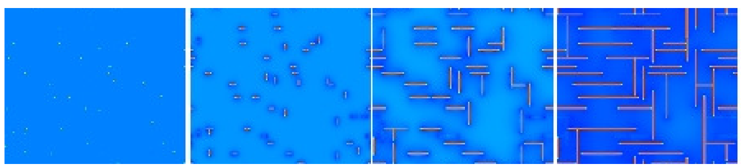
Art Ramirez

Thank you!

Interesting reading follows…

NHMFL Open House

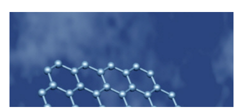
lhaworth@nsf.gov
http://www.nsf.gov/materials



Defects and Fluctuations in Low Dimensional Condensed Matter

H.A. Fertig, Indiana University (Bloomington), DMR-0454699

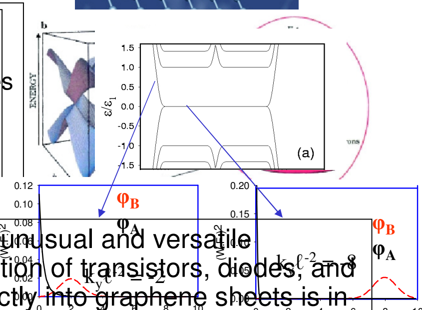
Observing "Relativity" in Condensed Matter: The Remarkable Electronic Properties of Graphene

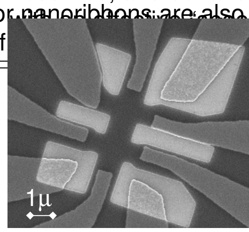


Graphene is a single sheet of graphite, the basic material used in pencils. It has recently become possible to fabricate this in single, two-dimensional sheets.

The electronic structure of graphene has a remarkable form that guarantees electrons always move at the same speed, regardless of their energy. Their low-energy description bears a close resemblance to (massless) neutrinos, and behave *relativistically*, although … "speed of light" that is 100 … true speed of light.

One consequence of this is that graphene does not conduct electricity the same way as standard semiconductors. Its electronic properties can be adjusted by cutting the sheet along different symmetry directions, or by manipulation of the sample width. Current carrying states for nanoribbons are also unique in the presence of …





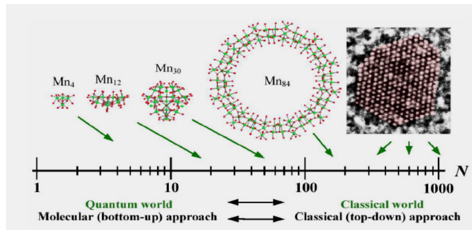
Because of these unusual and versatile properties, fabrication of transistors, diodes, and other devices directly into graphene sheets is in principle possible, opening exciting avenues for new concepts in ultrasmall electronic devices and integrated circuits.

Quantum Effects in Single Molecule Magnets

PIs: G. Christou, N. Dalal, S. Hill, A. D. Kent, D. N. Hendrickson

Inst: NYU, U FL, FSU, UCSD DMR-0103290

This project focuses on the synthesis and study of molecules that contain a small number of metal atoms, such as 12 manganese ions, that lock their individual magnetic moments together to form a larger and coherent "nano-magnet". The resulting moment of the molecule, unlike that of a single ion, is potentially large enough to detect and to use in an electronic device to process or store information. Miniaturization of magnetic devices to this size is critical to advances in information processing, which is an important industry in the United States. Of particular interest is that magnetic properties at this size scale are inherently quantum mechanical in nature. For example, molecules can reverse their magnetization direction by quantum tunneling (QTM), which is poorly understood. This research project has lead to a better understanding of the interactions that produce tunneling and the discovery of new quantum phenomena in magnetic molecules. Highlights include:



Molecules synthesized and studied in this project in our bottom-up approach to nanomagnetism. The largest molecule (Mn_{84}) is at the scale of Co nanoparticles realized by conventional methods.

- Chemical control of quantum tunneling of the magnetization (Nature 2002)
  - Subtle changes in molecular structure have been shown to have a dramatic effect on QTM.
- Quantum coherence in SMMs (Physical Review Letters 2004, Science 2003)
  - Experiments have probed the time scales over which the magnetization dynamics is coherent, which is of great fundamental and practical interest.
- Mechanisms that produce magnetic tunneling (Physical Review Letters 2003)
  - The interactions that produce tunneling have been determined in the first and most widely studied SMMs, Mn_{12}-acetate.

Top-Cited Paper in Physics

(1/07 for past 2 years)

http://www.in-cites.com/hotpapers/2007/jan07-phy.html

Citations: 164

Title: OBSERVATION OF THE SPIN HALL EFFECT IN SEMICONDUCTORS

Authors: KATO YK; MYERS RC; GOSSARD AC; AWSCHALOM DD

Source: SCIENCE 306 (5703): 1910-1913 DEC 10 2004

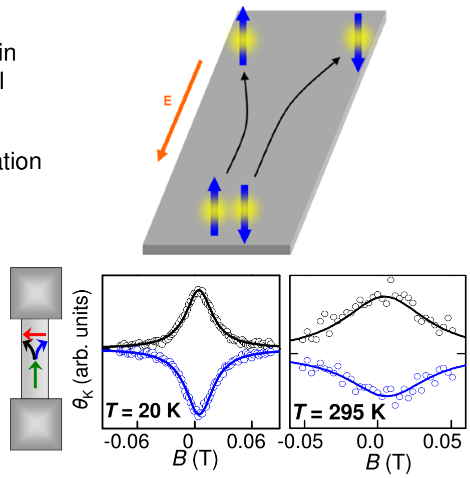
Addresses: Univ Calif Santa Barbara, Ctr Spinatron & Quantum Computat, Santa Barbara, CA 93106 USA.

Field: PHYSICS

Current-induced polarization and the spin Hall effect at room temperature

D.D. Awschalom, University of California – Santa Barbara
N. Samarth, Pennsylvania State University
DMR-0305223, DMR-0305238

- Unexpected observation of electrical spin generation in materials with weak internal magnetic fields.
- Spatial imaging of electron spin polarization using Kerr rotation microscopy.
- Bulk electron spin polarization due to electric currents in ZnSe up to room temperature.
- Evidence of extrinsic spin Hall effect in ZnSe from liquid helium to room temperature: pathway towards applications.

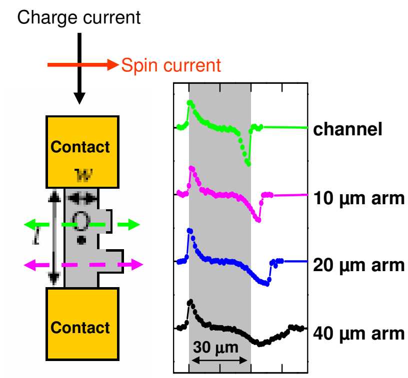


N. Stern *et al.*, *Phys. Rev. Lett.* **97**, 126603 (2006)

All-electrical generation of spin currents in semiconductors

D.D. Awschalom, University of California – Santa Barbara
DMR-0305223

- Electrical creation and control of electron spins in devices important for spin-based information processing.
- Generated spin polarization and currents on-chip with conventional semiconductors… no magnets or magnetic materials required.
- Spatially-resolved pure electron spin currents using the recently-discovered spin Hall effect.
- Spin currents transported ~ 50 microns, far greater than today's feature sizes in electronic.



Vanessa Sih *et al.*, *Phys. Rev. Lett.* **97**, 096605 (2006)

Spin transport studies in band and interface tailored materials: towards total spin polarization for spin electronics

Jagadeesh S. Moodera, MIT, DMR - 0504158

i) A novel ferromagnetic semiconductor:

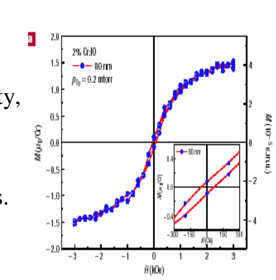
- A novel magnetic semiconductor has been developed. that may greatly increase the computing power, storage capacity, and flexibility of future electronic devices.
- The magnetic semiconductor material created by us is indium oxide with chromium- and oxygen-induced defects.
- This new material can be used to injects spins of a given orientation into the semiconductor such as silicon. These spins then travel through the semiconductor and are read by a spin detector.
- Spin injection at room temperature and its transparency shows the new material's potential for application.
- Published in Nature Materials (April 2006).

Media coverage of this work. A few examples are given below:

http://economictimes.indiatimes.com/articleshow/1593432.cms

http://www.elecdesign.com/Articles/Index.cfm?ArticleID=13244

Also in MIT TechTalk and website and in IEEE Spectrum



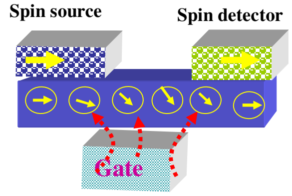


Fig. 1 The magnetic properties of a Cr doped In2O3 film at 300K and the schematic of a spin based device – SpinFET

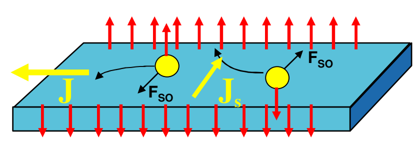
Many body effects in electronic dynamics and transport

Giovanni Vignale, University of Missouri-Columbia, DMR-0313681

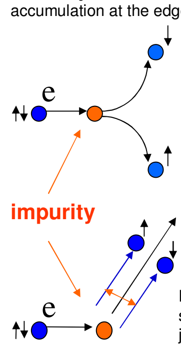
Electron-electron interaction in the Spin Hall Effect

The Spin Hall Effect is the generation of a lateral spin current from a regular electric current. It attracts great interest as a method to separate electrons of opposite spin by purely electrical means (see Figure). The main driving mechanism for the Spin Hall Effect is the scattering of electrons by impurities in the presence of spin-orbit interaction. The figure shows the two main processes through which impurities separate the spins: they are known as skew scattering and side jump.

In addition, the magnitude of the spin current is strongly influenced by the Coulomb interaction between the electrons. When electrons of opposite spin travel in opposite directions they exert a force on each other, tending to reduce the relative motion. This is the phenomenon of the spin Coulomb drag and we have studied its impact on the Spin Hall Effect.



Spin Hall Effect: the regular current (J) drives a spin current (J_s) across the bar resulting in a spin accumulation at the edges.



Skew scattering

More spin up electrons are deflected to the right than to the left (and viceversa for spin down)

Side Jump

For a given deflection, spin up and spin down electrons make a side-jump in opposite directions.

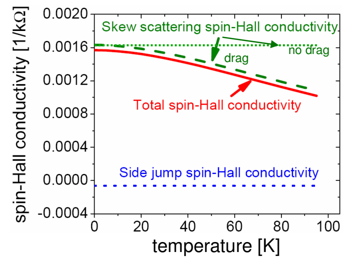
How to distinguish different contributions to the spin Hall effect

Spin Coulomb Drag

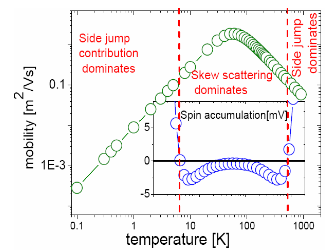
Our results are summarized in the top figure on the right. We found that the spin Coulomb drag *reduces* the skew-scattering contribution. The contributions with and without Coulomb drag are shown by the dotted and the dashed green lines respectively. The side-jump contribution (blue dashed line) remains unaffected. The figure also shows the typical magnitude of the two contributions at different temperatures in a clean GaAs spin Hall bar.

A crucial experiment

We propose an experiment to distinguish the skew-scattering and side-jump contributions. We observe that the side jump and the skew scattering have opposite signs. But the side jump is independent of temperature while the skew scattering is directly proportional to the electronic mobility - a measure of how fast the electron can drift in an electric field - which in turn is strongly dependent on temperature (green circles on the right). Hence we expect a transition from a skew-scattering-dominated to a side-jump-dominated regime as the temperature is reduced. A change in sign of the spin accumulation will reveal the transition.

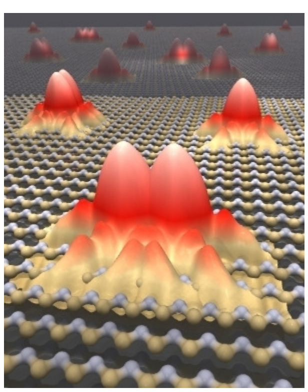


E. Hankiewicz and G. Vignale, Phys. Rev. B 73, 115339 (2006)



E. Hankiewicz and G. Vignale and M. Flatte', cond-mat/0603144

"Atom-by-Atom Substitution of Mn in GaAs and Visualization of their Hole-Mediated Interactions," D. Kitchen, A. Richardella, J.-M. Tang, M. E. Flatté, A. Yazdani, *Nature* **442**, 436 (2006).



SPINTRONICS AT THE ATOMIC LEVEL
A positive spin on GaAs seminconductors
A novel technique developed by our group uses a scanning tunneling microscope (STM) to substitute atoms into a semiconductor one atom at a time. This technique has been used to assemble a magnetic semiconductor, manganese-doped gallium arsenide (Ga1-xMnxAs), atom by atom. This work was recently published as the cover article in Nature as a *Letter* titled, "Atom-by-Atom Substitution of Mn in GaAs and Visualization of their Hole-Mediated Interactions." More details about these experiments can be found under our group's research of Single Spins.

Coherence, correlation, and disorder in complex materials and nanoscale devices

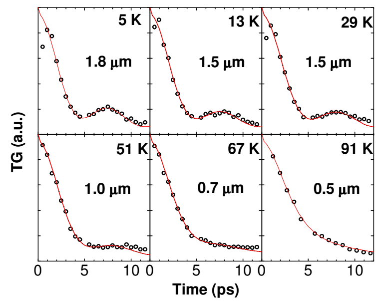
Joel E. Moore, UC Berkeley, DMR-0238760

Spin ordering and transport:

One of the fundamental differences between spin currents and charge currents is **"spin drag":**[1] collisions between spin-up and spin-down electrons tend to equalize their currents, even on short time scales when electron spin is conserved.

Understanding new experiments on spin drag required development of a kinetic-theory approach[2] incorporating electron correlations and potential scattering to understand the ballistic-diffusive crossover in spin transport.

Spin grating decay vs. time
(red curve=theory)

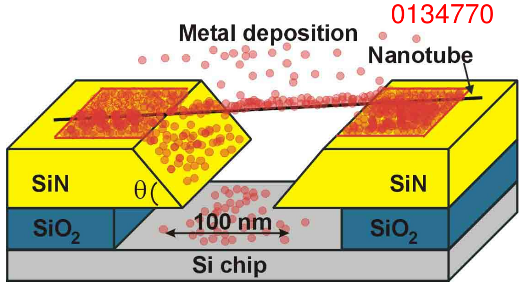


1. I. D'Amico and G. Vignale, PRB 68, 45307 (2003).

2. C. P. Weber, N. Gedik, J. E. Moore, J. W. Orenstein, J. Stephens, and D. D. Awschalom, *Nature*, to appear.

CAREER: Quantum Properties of Ultrasmall Homogeneous Superconducting Nanostructurees

Alexey Bezryadin, University of Illinois at Urbana-Champaign, DMR-0134770



Extremely thin nanowires (about 5–10 nm; a nanometer is one-billionth of a meter) have been made by our group using the "molecular templating" method illustrated in the drawing. Simply put, a single molecule (a carbon nanotube or a molecule of DNA) is positioned across a trench in a substrate and decorated with a few atomic layers of metal, thus forming a very thin nanowire.

Using molecular templates (see figure), we have fabricated record-thin superconducting wires. In general, superconductors are used in magnetic resonance imaging systems, magnetic-levitation railways and trains, and in so-called SQUID systems, which, among other things, can detect tiny variations in the magnetic field of a living brain. Eventually, superconducting wires might be used to build power lines, such that they could carry electrical energy long distances with almost no loss. Now, as reported in the Sept. 29, 2006 issue of *Physical Review Letters*, our group has found a highly unusual phenomenon: a magnetic field enhances the maximum possible (i.e. "critical") value of the lossless current (i.e. the "supercurrent") that can flow though a nanowire. We have not only discovered this unusual behavior in which ultra-narrow wires show increased superconductivity as they are exposed to higher magnetic fields, but we have also developed a theory that explains it, in collaboration with P. Goldbart's theory group.

Novel quantum interference device made of DNA-templated superconducting nanowires

Alexey Bezryadin, University of Illinois at Urbana-Champaign, DMR-0134770

Strands of DNA have been used as tiny scaffolds to create superconducting nanodevices that demonstrate a new quantum interference phenomenon. These nanowire quantum interference devices (NQIDs), which comprise a pair of suspended superconducting wires as thin as a few molecular diameters (5 nm to 20 nm), could be used to measure magnetic fields and to map out the phase of the order parameter in regions of superconductivity.

The figure at the right shows an artist's conception of the NQID. Two strands of DNA have been suspended over a trench cut into a substrate and then sputtered with a superconducting alloy to create the nanowires and leads. Such novel metallic nanodevices can be integrated into large arrays using well-known self-assembly properties of DNA molecules.

Reference: D. Hopkins et al., *Science* **308**,1762 (2005)

Ohm's law in smart materials

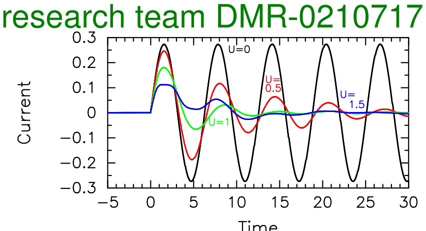
PI's: J. K. Freericks (Georgetown), A. Y. Liu (Georgetown), and B. A. Jones (IBM)

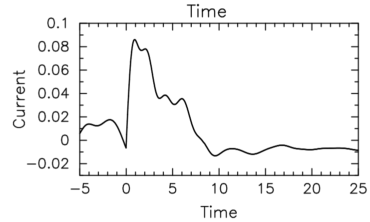
Nanotechnology interdisciplinary research team DMR-0210717

Ohm's law (V=IR) where the voltage is equal to the product of the current and the resistance is one of the best known formulas in physics. In our work, we examine how this law is violated in smart materials composed of systems where the electron-electron repulsion is so strong that the electrons avoid each other in a complicated quantum-mechanical dance.

In nearly all materials, the atoms that compose it are ordered in a periodic arrangement. In this case, when a battery is attached to the material, it creates an oscillating current called a Bloch oscillation. As the electrons scatter off of themselves and off of defects in the material, the oscillations die off. We calculate how these regular oscillations decay and how they become irregular as the material undergoes a transition from a metal to an insulator due solely to the mutual repulsion of the electrons.

For more details see http://www.physics.georgetown.edu/~jkf/nirt.html





Top: Oscillations in the current for a perfect conductor (U=0), and for materials that have increasingly stronger scattering (labeled by increasing U).
Left: Irregular oscillations in the insulator that is created by very strong electron-electron repulsion.

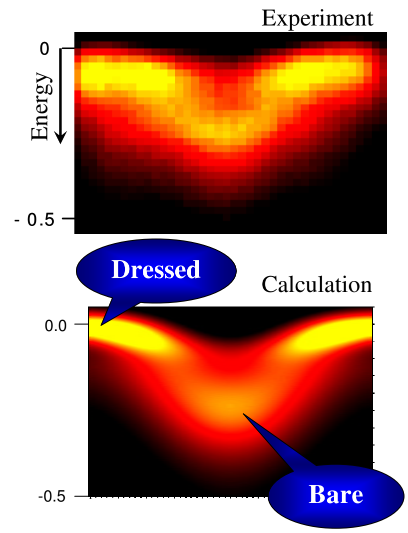
Electron-Phonon Coupling at a Silicon Surface

Franz Himpsel, UW-Madison DMR-0240937
Synchrotron Radiation Center DMR-0537588

When an electron approaches zero energy, it slows down and drags nearby atoms with it. It becomes a dressed electron, which is heavier than bare electrons at high energy.

This effect has now been found at a semiconductor surface, where it is possible to identify the electrons and atoms that are involved.

Controlling electron-phonon coupling at a surface may lead to new electronic materials.



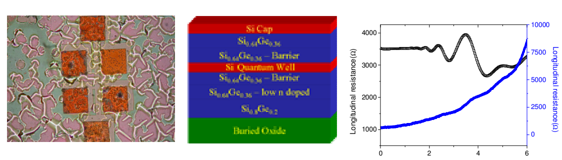
Barke et al., Phys. Rev. Lett. **96**, 216801 (2006)

Elastically Relaxed Free-standing Strained-Si Nanomembranes‡

Michelle M. Roberts, Levente J. Klein, Don E. Savage, Keith A. Slinker, Mark Friesen, *George Celler, Mark A. Eriksson, Max G. Lagally
University of Wisconsin-Madison, Madison, Wisconsin 53711, USA
*Soitec USA, 2 Centennial Dr, Peabody, MA 01960

Strain in silicon is useful for creating both classical and quantum electronic devices. Researchers at UW-Madison and Soitec USA have demonstrated that strain can be created in silicon membranes by a purely elastic process that avoids the creation of defects. In this technique, silicon-germanium is grown epitaxially on a silicon-on-insulator substrate. This multilayer system is then released into a liquid solution, allowing the membrane to share strain between its various layers. Such membranes can then be re-deposited for further processing or applications. In carefully designed structures, the end result is a strained silicon film on a new substrate. Measurements after release and re-deposition of such membranes demonstrate the observation of desired quantum effects that require strained silicon. An advantage of this new approach is that the multilayer silicon-germanium nanomembranes can be deposited on a wide variety of substrates, ranging from traditional semiconductors to plastics. Thus, high quality strained silicon can be placed on new substrates for applications.

Primary support for this project was provided by NSF through the ITR (DMR-0325634), MRSEC (DMR-0520527), and graduate fellowship programs.

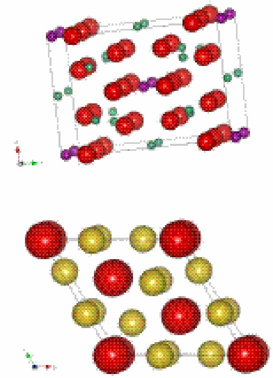


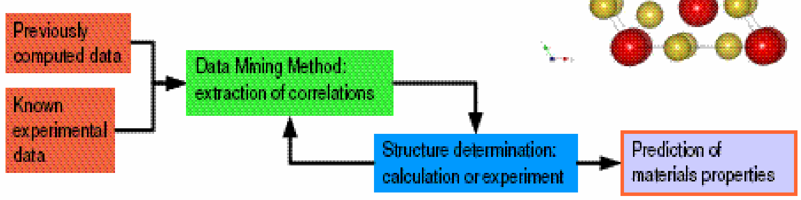
(Left) Transferred membrane containing a patterned Hall bar. (Center) Growth layers for a coherently strained heterostructure. (Right) Low temperature resistance measurement as a function of magnetic field. The large upward curvature (blue line) before release is a result of too little strain in the silicon, as expected before strain sharing is achieved. After the membrane is released and strain sharing occurs, a flat curve with increasing oscillations is observed (black line), characteristic of good quantum well confinement. Such confinement is beneficial for low temperature quantum devices and room temperature classical electronics.

Predicting crystal structure: combining data mining with quantum mechanics

Prof. Gerbrand Ceder, MIT, Prof. Dane Morgan, UW-Madison
(DMR-0312537)

Virtual Materials Design is the design of new materials through computational modeling starting from the basic laws of physics, and holds the potential to accelerate the rate at which new materials are developed for a wide range of applications. One critical problem in the virtual materials design process is determining the most stable arrangement of the atoms in a material. This structural information is needed before reliable predictions of the material's properties can be made. We have developed a method which learns rules to predict structure from the large body of historical information on existing materials and uses it to predict the structure of new materials in a highly efficient way.





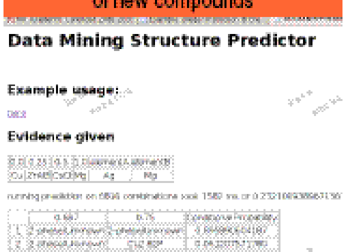
Predicting crystal structure: combining data mining with quantum mechanics

Prof. Gerbrand Ceder, MIT, Prof. Dane Morgan, UW-Madison
(DMR-0312537)

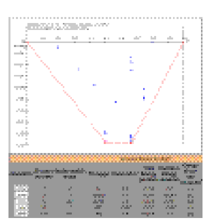
http://datamine.mit.edu

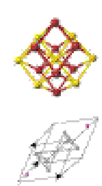
The results of our structure prediction research are now available on-line, providing public access to the output of over 14,000 ab initio calculations. In addition, a beta-stage structure predictor is now available.

make predictions about the structure of new compounds



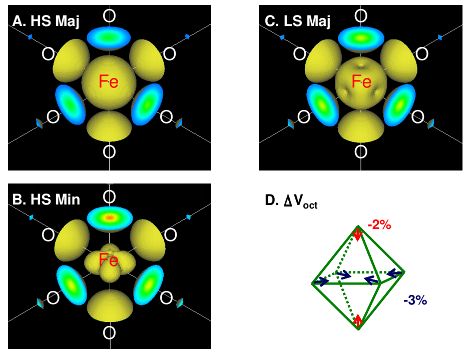
view the results of ab initio calculations





Institute for the Theory of Advanced Materials in Information Technology: James R. Chelikowsky (Texas), Yousef Saad and Renata Wentzcovitch (Minnesota), Steven Louie (UC Berkeley) and Efthimios Kaxiras (Harvard) (DMR- 0551195): Spin transition in complex oxides under pressure

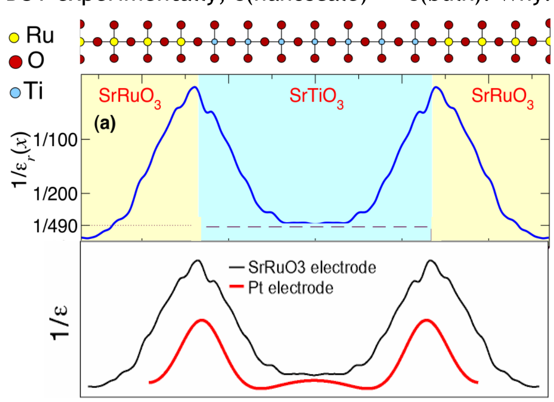
Fe-Mg oxides may undergo a high spin (HS) to low spin (LS) transition under pressure (23-135 GPa). Previous first principles methods have failed to describe this phenomenon. Using a new rotationally invariant formulation of density functional theory (LDA+*U*), we were able to describe successfully this transition in the low solute concentration for the oxide: magnesiowüstite (Mw), $(Mg_{1-x}Fe_x)O$, ($x < 0.2$). We show that the HS/LS transition goes through an insulating (semiconducting) intermediate mixed spins state without discontinuous changes in properties, as seen experimentally. These encouraging results open for exploration by first principles a new class of spin related phenomena.



Charge densities around a ferrous iron in magnesiowüstite. Isosurface charge densities with ρ = 0.3 e/Å^3 for majority (A) and minority HS (B), and majority/minority LS (C). Polyhedral volume collapse across the spin transition (D). Six caps surrounding the ferrous ion belong to oxygens.

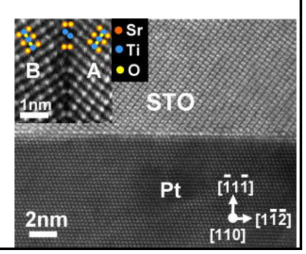
Existence and origin of "dielectric dead layer" in nanoscale capacitors
M. Stengel and N.A. Spaldin, cond-mat/0511042 and Nature (in press)

Nanoscale capacitors with high dielectric constant ε needed for device miniaturization BUT experimentally, ε(nanoscale) << ε(bulk). Why? Calculate ε from first-principles:



Intrinsic "dielectric dead layer" at ideal $SrTiO_3/SrTiO_3$ interface; dead layer is reduced for Pt electrodes

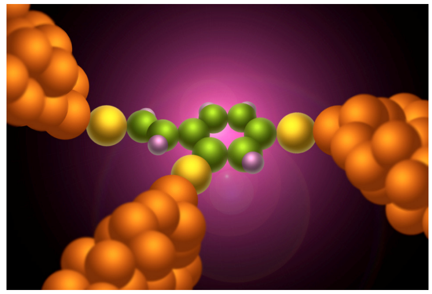
Need improved $Pt/SrTiO_3$ interfaces and accurate characterization, as in this high-resolution image from Stemmer et al. (APL 88, 131914 (2006))



Quantum Transport and Metallic Nanocohesion

Charles A. Stafford, University of Arizona, DMR-0312028

- A new device concept, the Quantum Interference Effect Transistor (QuIET), was proposed.
- In the "off" state, current is blocked by perfect destructive interference stemming from *molecular symmetry*.
- Current turned "on" by introducing decoherence/scattering from a third lead.
- Current controlled by regulating interference, *not* by raising/lowering an energy barrier.



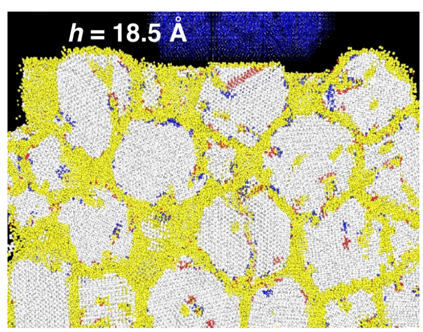
Artist's conception of a QuIET based on sulfonated vinyl benzene. Colored spheres represent individual carbon (green), hydrogen (purple), sulfur (yellow), and gold (gold) atoms. Voltage applied to the leftmost contact regulates current between the other two.

David M. Cardamone, CAS & S. Mazumdar, *Nano Letters* (November 2006 cover article).[1]

Mechanical Response of a Nanocrystal

Izabela Szlufarska, University of Wisconsin DMR-0512228
P. Vashishta, R. Kalia, A. Nakano, USC DMR-0427188
W. Goddard, T. Cagin, P. Meulbroek, M. Ortiz, A. van Duin, CalTech DMR-0427177
A. Grama, Purdue DMR-0427540

- **MD simulation:** nanoindentor into nanocrystalline silicon carbide (n-SiC).
- **n-SiC**: high hardness and toughness.
- **Hardness:** simulation (19 million-atoms) and experiment agree.
- **Discovery:** crossover from intergrain to intragranular response with increasing depth.
- **Crossover:** arises from the coexistence of hard crystalline grains (white) and soft amorphous intergranular phases (yellow).
- **Mechanical response:** intriguing interplay between ordering (blue) and disordering (red).



"A crossover in the mechanical response of nanocrystalline ceramics"
Science **309**, 911 (2005)

High-performance transparent inorganic–organic hybrid thin-film n-type transistors

LIAN WANG, MYUNG-HAN YOON, GANG LU, YU YANG, ANTONIO FACCHETTI AND TOBIN J. MARKS*
Department of Chemistry and the Materials Research Center, Northwestern University, Evanston, Illinois 60208-3113, USA
*e-mail: t-marks@northwestern.edu

(See Nature Mater. **5**, 893, 2006)

Published online: 15 October 2006; doi:10.1038/nmat1755

"The results suggest new strategies for achieving 'invisible' optoelectronics"

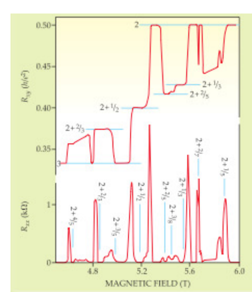
Novel Ordered States of Electrons

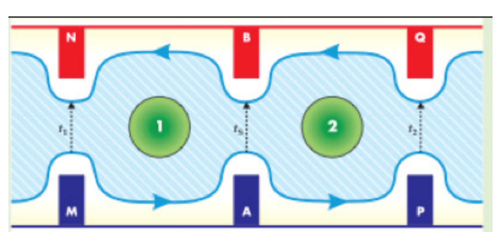
Chetan Nayak, UCLA, DMR-0411800

•With M. Freedman and S. Das Sarma, the PI proposed a device based on a possible new state of matter (non-Abelian FQH state)

•A step towards a topological quantum computer =>

Exploit robustness of topological phases to perform fault-tolerant quantum computation.





With M. Freedman and K. Walker, a quantum computing architecture built around this device.

With P. Fendley and M.P.A. Fisher, analyzed the properties of point contacts in non-Abelian quantum Hall states, the basic building blocks of such devices.

With several collaborators, analogous set-up in cold-atom systems proposed.

Young Scientists Trained:

C. Bena, I. Dimov, W. Bishara

Outreach:

Public Dialog Lecture:
"Electrons, Topology, and Quantum Computation" (Aspen, CO.)

This work has been featured in *Scientific American* and *Physics Today*
The supporting science:

S. Das Sarma, M. Freedman, C. Nayak, Phys. Rev. Lett 94, 166802 (2005).
M. Freedman, C. Nayak, K. Walker, Phys. Rev. B 73, 245307 (2006).
P. Fendley, M.P.A. Fisher, and C. Nayak, Phys. Rev. Lett. 97, 036801 (2006).
S. Tewari, S. Das Sarma, C. Nayak, C. Zhang, P. Zoller, quant-ph/0606101.

AAAS Newcomb Cleveland Prize 2006
Jason R. Petta, Alexander C. Johnson, Jacob M. Taylor, Edward A. Laird, Amir Yacoby, Mikhail D. Lukin, Charles M. Marcus, Micah P. Hanson, Arthur C. Gossard for the research article "Coherent Manipulation of Coupled Electron Spins in Semiconductor Quantum Dots," published online in *Science* Express 1 September 2005, published in print 30 September 2005, pp. 2180-2184.

This paper shows a system in which two closely spaced gallium arsenide quantum dots each holds an electron. The spins of the electrons are managed by an imposed magnetic field and also by electrostatic control provided by electrodes spanning the two dots. The electron on each dot combine to form "singlet spin state" where the spins are anti-parallel, but this state remains coherent for only about 1 nanosecond because of the influence of the neighboring nuclear spins in the crystal. Ingeniously, the authors were able to exchange electrons in a way that effectively eliminated influence from the crystal nuclei and restore the singlet state. The swaps, between the singlet-state anti-parallel alignment and the triplet-state parallel alignment, could maintain coherence for more than one microsecond, which is sufficient to offer promise in the design of spin-coded quantum computation.

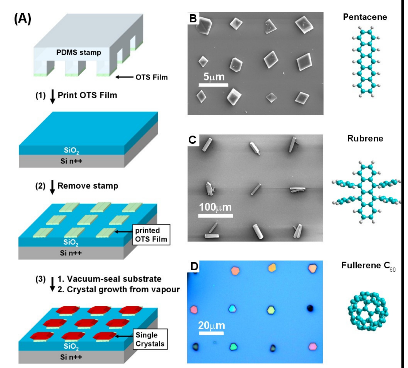
Patterning of Large Arrays of Organic Semiconductor Single Crystals

Alejandro L. Briseno[1,2], Stefan C.B. Mannsfeld[1], Mang M. Ling[1], Shuhong Liu[1], Ricky J. Tseng[2], Colin Reese[1], Mark E. Roberts[1], Yang Yang[2], Fred Wudl[2], Zhenan Bao[1], [1]Stanford University, [2]UCLA,

Supported by the Center on Polymer Interfaces and Macromolecular Assemblies, a NSF Materials Research Science and Engineering Center, NSF DMR-0213618, and also AFOSR F49620-03-1-0101, Bell Labs Graduate Fellowship, and DFG Postdoc Fellowship

We developed a method for effectively fabricating large arrays of single crystals of a wide range of organic semiconductor materials directly onto transistor source-drain electrodes. Field-effect transistors made of single organic crystals are ideal for studying the charge transport characteristics of organic semiconductor materials. Their outstanding device performance, relative to that of transistors made of organic thin films, makes them also attractive candidates for electronic applications such as active matrix displays and sensor arrays. The only approach currently available for creating single crystal devices is manual selection and placing of individual crystals—a process prohibitive for producing devices at high density and with reasonable throughput. We fabricated large arrays of high-performance organic single-crystal field effect transistors with mobilities as high as 2.4 cm^2/Vs and on/off ratios greater than 10^7, and devices on flexible substrates that retain their performance after significant bending. These results suggest that our fabrication approach constitutes a promising step that might ultimately allow us to utilize high-performance organic single crystal field-effect transistors for large-area electronics applications.

Nature, vol 466, December 14, 2006, 913-917



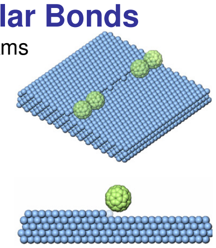
A, Schematic outline of the procedure: print with polydimethylsiloxane (PDMS) stamps with relief features that are inked with a thick octadecyl-triethoxysilane (OTS) film and then press onto the substrates, place patterned substrate in vacuum-sealed tube in a temperature gradient furnace tube with the organic semiconductor source material for growth of patterned single crystals. **B,** Patterned single crystal arrays of Pentacene **C,** Rubrene **D,** C60.

University of Maryland NSF-MRSEC Highlight:

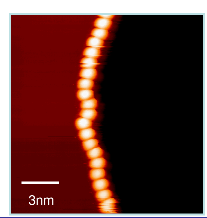
Metal Electrodes Fluctuate under Molecular Bonds

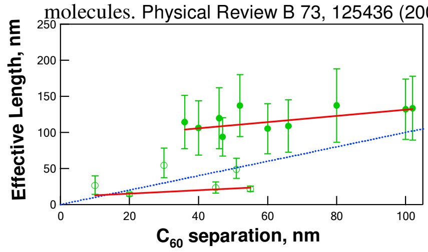
C. Tao, T.J. Stasevich, T.L. Einstein and E.D. Williams

DMR-0520471



Metal-molecule contacts play a key role in defining electron transport in molecular electronics. However, the possibility of structural motion, e.g wandering atoms on the metal electrode, may lead to stochastic behavior in the "device" properties. A model system to investigate this issue is provided by the strong bonding of C60 molecules to step edges on a Ag surface. When free, the step edges move dynamically at room temperature via hopping of atoms along the step edge. If C_{60} bonding restricted atomic motion, it would limit the effective length of the step to the distance between C_{60} molecules. By fabricating step configurations with different C_{60} separations, we show that there is no variation in the effective length, thus Ag atoms continue to fluctuate in position, despite the presence of the bound molecules. Physical Review B 73, 125436 (2006)





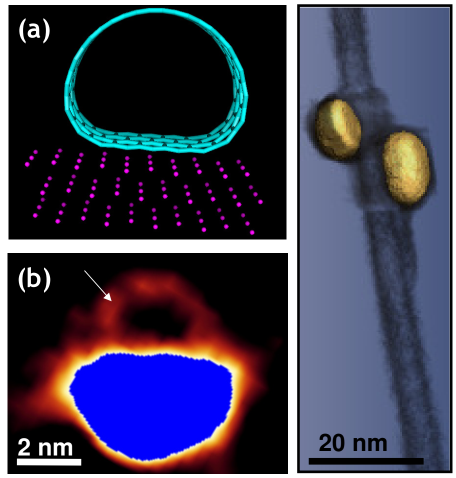
Evolution of structure

Above: Scale drawing and STM image of C_{60} molecules bound to a step edge on Ag(111).

Left: Measured effective length of the fluctuating step shows no significant variation with the separation between C60 molecules bound to the step. Hindered atomic motion would have yielded the dependence shown as the blue line.

Do not bend, fold or mutilate

- Carbon nanotubes are hollow tubes made from single sheets of carbon atoms. Along the length of the tube they can be excellent electrical conductors, and they are also the stiffest known material. However, just like a drinking straw, they can be easily deformed or pinched in a radial direction. Attaching electrical contacts to the tube has always proved challenging – some contacts are good, others a thousand times worse. The first 3-dimensional images of contacts between a metal and a nanotube now explain why: bad contacts squish the tube and disturb the electron flow. Good contacts will wrap around the tube without deforming it.



(a) Theoretical simulation of a no-longer round nanotube deformed by contact with a palladium surface. (b) Experimental image of a nanotube (white arrow) in contact with a palladium-gold contact, showing the deformation from a circular tube cross section.

- Judy J. Cha and D. Muller (IRG-1)
- Jean-Francois Briere and T. Arias (IRG-3)

14-2

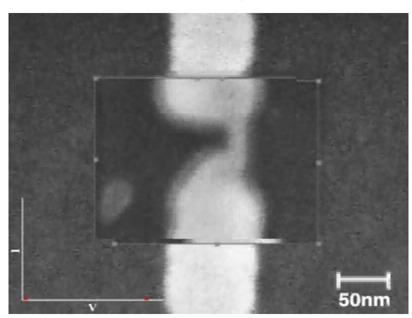
Electron Transport in Nanostructures and Single Molecules

Dan Ralph, Cornell University, DMR-0244713

We are inventing techniques to incorporate single molecules into electrical circuits and measure their properties.

The size scale of molecules is so small that it is very challenging to make well-controlled, reproducible devices, or to even find ways to image devices during the fabrication process. One of our group's important recent innovations is that we have developed experimental techniques to watch and control nanoscale wires as we sculpt them into desired shapes with an electrical current.

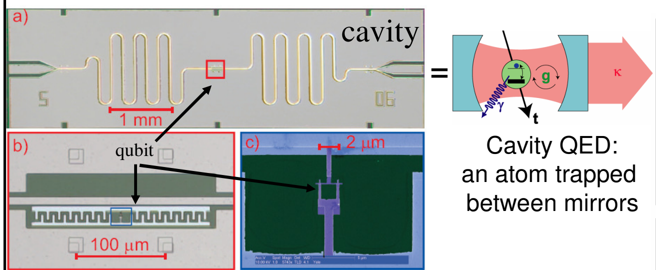
(click picture to watch movie)

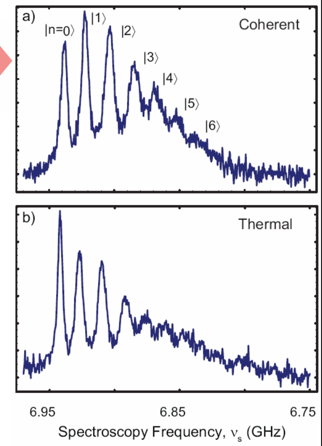


This movie shows a nanoscale gold wire with a narrow neck as we pass electrical current to sculpt the wire, break it, and form a controlled gap into which we can connect single molecules. The graph on the left shows a simultaneously-measured current-voltage curve. The current drops when the wire narrows and then eventually breaks.

Circuit Quantum Electrodynamics: Resolving Photon Number States in a Superconducting Circuit

R.J. Schoelkopf and S.M. Girvin; *Yale University, ITR/DMR-0325580*



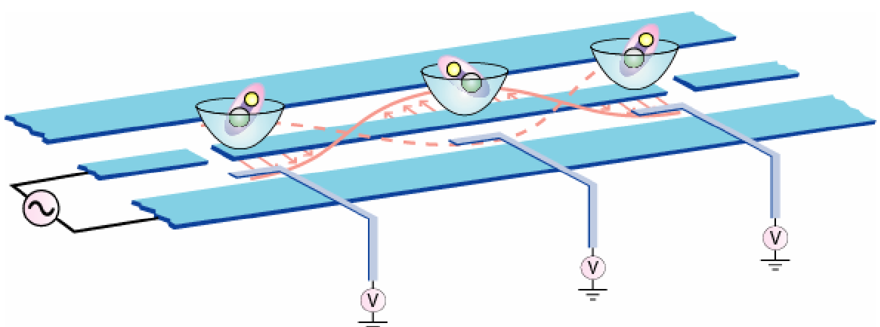


Integrated circuit in which a superconducting "qubit," or artificial atom, is coupled to microwave photons trapped in a super-conducting transmission line "cavity," in direct analogy with the field of cavity quantum electrodynamics (cavity QED) in quantum optics.

First observation of individual photon number states of the cavity via qubit spectroscopy in the strong dispersive coupling regime.

The Molecule Chip: An All-Electrical Interface for Isolated Quantum Particles

D. DeMille and R.J. Schoelkopf; *Yale University*
Center for Quantum Information Physics, ITR/DMR-0325580



Artist's conception of a proposed new device, the "molecule chip". Microfabricated electrical traces, with appropriate applied voltages, can be used to trap polar molecules just above the surface of a chip. The trapping sites are located within the electrodes of a superconducting microwave stripline resonator. With this system, it is possible to achieve a strong, quantum-mechanically coherent coupling between molecules and microwave photons. This coupling will enable an unprecedented level of control over quantum information, by encoding into the internal states of the molecules.