2014 Workshop on Innovative Nanoscale Devices and Systems

WINDS

Booklet of Abstracts

Edited by

Viktor Sverdlov
Berry Jonker
Koji Ishibashi
Stephen M. Goodnick
Siegfried Selberherr

Hapuna Beach Prince Hotel
Kohala Coast, Hawaii, USA

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The **Workshop on Innovative Nanoscale Devices and Systems** (WINDS) is a 4½ day meeting with morning and evening sessions, and with afternoons free for *ad hoc* meetings and discussions among participants. WINDS follows the tradition and format of AHW (Advanced Heterostructure Workshop). In 2008, there was a transition as the workshop name morphed from AHW to AHNW to WINDS in order to attract more participation from industrial labs. The format of each session involves one or two overview presentations plus lively discussion (about 15 minutes for each paper) based on recent data. To ensure enough time for discussion, short presentation of data is encouraged. Each participant is expected to engage in these discussions and is strongly encouraged to bring three to four overhead transparencies or a PC with PowerPoint files showing most recent results that can be incorporated into the discussions. Titles, introductions, summary, and acknowledgements are strictly discouraged. The total number of participants will be limited to around 80 to keep the discussions lively in the single session.

Conference Organization

General Chair
Viktor Sverdlov, Technical University Vienna, Austria
sverdlov@iue.tuwien.ac.at

US Co-Chair
Berry Jonker, NRL, USA
berry.jonker@nrl.navy.ml

Europe Co-Chair
Siegfried Selberherr, Technical University Vienna, Austria
Selberherr@TUWien.ac.at

Japan Co-Chair
Koji Ishibashi, RIKEN, Japan
kishiba@riken.jp

Local Arrangements
Stephen M. Goodnick, Arizona State University, USA
stephen.goodnick@asu.edu

November 30th (Sunday)

15:00-18:00 Registration (Breezeway-Kohala)

18:00-20:00 Welcome Reception (Poolside)

December 1st (Monday)

8:50–9:00 Opening

Majorana and Parafermions (Berry Jonker, NRL)

10:30-11:00 Coffee Break

Search for Majorana and more (Matthew Gilbert, Univ. Urbana Champaign)

December 1st (Monday) continued

December 2nd (Tuesday)

Topological Insulators (Alexander Balandin, UC Riverside)

10:30-11:00 Coffee Break

Topological Insulators and Devices (Asen Asenow, Univ. of Glasgow)

December 2nd (Tuesday) continued

2D Materials (Leonard Register, UTexas, Austin)

13:00-21:00 *Ad hoc* Session

December 3rd (Wednesday)

CMOS Scaling and more (Stephen Goodnick, Arizona State Univ.)

10:30-11:00 Coffee Break

December 3rd (Wednesday) continued

Spintronics 1 (Siegfried Selberherr, TU Wien)

Molecular Electronics (Siegfried Selberherr, TU Wien)

13:00-18:30 *Ad hoc* Session

18:30-21:00 Banquet (Courtyard)

December 4th (Thursday)

Graphene and Nanotubes (Koji Ishibashi, RIKEN)

10:30-11:00 Coffee Break

Graphene: Growth and Applications (David Ferry, Arizona State Univ.)

12:45-19:00 *Ad hoc* Session

December 4th (Thursday) continued

Molecular Electrons and Simulations (Viktor Sverdlov, TU Wien)

Light Sources, Photonics, and Photovoltaics (Eiji Saitoh, Tohoku Univ.)

December 5th (Friday)

Spintronics 2 (Igor Zutic, Univ. at Buffalo)

10:30-11:00 Coffee break and Closing

Non-Abelian Anyons in Condensed Matter: Majorana to Parafermions

Matthew J. Gilbert

Department of Electrical and Computer Engineering
Micro and Nanotechnology Laboratory
University of Illinois – Urbana-Champaign
208 N. Wright Street
Urbana, IL 61801, USA

Tel: +1 217 333 3064
email: matthewg@illinois.edu

It is a generally acknowledged fact that the semiconductor devices that comprise CMOS-based computing architectures consume far too much power. To this end, an extensive search has been underway for alternative methods to not only reduce the power consumed but to boost the overall computational power. One of the most promising alternatives to CMOS-based computing is the idea of topological quantum computing. Here carefully engineered quantum states are used to both store and manipulate quantum information in a manner that is both non-local and immune from disorder effects. The backbone of topological quantum computation is the Majorana fermion and its generalization the parafermion both of which are non-Abelian quasi-particles whose exchange statistics are neither fermionic nor bosonic in nature. In this talk, I will review the basic physical principles behind Majorana and parafermions as well as discuss some of the major theoretical and experimental efforts to find these elusive quasi-particles in condensed matter settings[1] focusing in particular on pairing three-dimensional time-reversal topological insulators with conventional s-wave superconductors[2]. I will conclude by discussing some of the future directions and open questions within this very interesting and dynamic field of condensed matter physics.

This work is supported by the Office of Naval Research and the National Science Foundation

1. A. Stern and N. H. Lindner, Science 339, 1179 (2013).
2. S. Y. Xu et al., Submitted to Nature Physics.

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Exotic Bound States in Low Dimensions: Majorana Fermions and Parafermions

Jelena Klinovaja

Department of Physics, Harvard University, Cambridge, Massachusetts 02138, USA,
Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland

email: klinovaja@physics.harvard.edu

In my talk, I will present recent results on exotic bound states in one-dimensional condensed matter systems that have attracted wide attention due to their promise of non-Abelian statistics useful for topological quantum computing. For example, Majorana fermions can emerge in a variety of setups in which either standard or synthetic spin-orbit interaction is present. Here, I will discuss candidate materials such as semiconducting Rashba nanowires [1-2], graphene nanoribbons [3], atomic magnetic chains or magnetic semiconductors [4]. At the same time, much effort is invested in identifying systems that host even more exotic quasiparticles than Majorana fermions that obey non-Abelian statistics of the Fibonacci type. Generating such quasiparticles is a crucial step towards a more powerful braid statistics that enables universal topological quantum computing. In my talk, I will discuss time-reversal invariant parafermions. This setup consists of two quantum wires with Rashba spin-orbit interactions coupled to an s-wave superconductor, in the presence of strong electron-electron interactions [5].

1. J. Klinovaja and D. Loss, Phys. Rev. B 86, 085408 (2012).
2. D. Rainis, L. Trifunovic, J. Klinovaja, and D. Loss, Phys. Rev. B 87, 024515 (2013).
3. J. Klinovaja and D. Loss, Phys. Rev. X 3, 011008 (2013); J. Klinovaja and D. Loss, Phys. Rev. B 88, 075404 (2013).
4. J. Klinovaja, P. Stano, A. Yazdani, and D. Loss, Phys. Rev. Lett. 111, 186805 (2013).
5. J. Klinovaja and D. Loss, Phys. Rev. B 90, 045118 (2014).

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Anyonics: Designing Exotic Circuitry with non-Abelian Anyons

David J. Clarke, Jason Alicea, and Kirill Shtengel

Department of Physics & Astronomy,
University of California, Riverside
CA 92521, USA

and

Institute for Quantum Information & Matter
California Institute of Technology, Pasadena
CA 91125, USA

Tel: +1 951 827 1058 Fax: +1 951 827 4529
email: kirill.shtengel@ucr.edu

Non-Abelian anyons are widely sought for the exotic fundamental physics they harbor as well as for their possible applications for quantum information processing. Currently, there are numerous blueprints for stabilizing the simplest type of non-Abelian anyon, a Majorana zero energy mode bound to a vortex or a domain wall. One such candidate system, a so-called "Majorana wire" can be made by judiciously interfacing readily available materials; the experimental evidence for the viability of this approach is presently emerging. Following this idea, we introduce a device fabricated from conventional fractional quantum Hall states, s-wave superconductors and insulators with strong spin-orbit coupling. Similarly to a Majorana wire, the ends of our “quantum wire” would bind "parafermions", exotic non-Abelian anyons which can be viewed as fractionalised Majorana zero modes.

I will briefly discuss their properties and describe how such parafermions can be used to construct new and potentially useful circuit elements which include current and voltage mirrors, transistors for fractional charge currents and "flux capacitors".

This research was supported by the NSF through grants DMR-1341822 and DMR-0748925 and by the DARPA QuEST program.

1. David J. Clarke, Jason Alicea and Kirill Shtengel, Nature Commun. 4, 1348 (2013).
2. David J. Clarke, Jason Alicea and Kirill Shtengel, to appear in Nature Phys.

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One Dimensional Parafermionic Phases and Topological Order

Aris Alexandradinata[1], Chen Fang[1,2,3], Matthew Gilbert[3,4], Nicolas Regnault[1,5], and B. Andrei Bernevig[1]

[1] Department of Physics, Princeton University, Princeton, NJ 08544, USA

[2] Department of Physics, University of Illinois, Urbana IL 61801, USA

[3] Microelectronics Nanotechnology Laboratory, University of Illinois, 208N Wright Street, Urbana, IL 61801, USA

[4] Department of Electrical and Computer Engineering, University of Illinois, Urbana, IL 61801, USA

[5] Laboratoire Pierre Aigrain, ENS-CNRS UMR 8551, Universites P. et M. Curie and Paris-Diderot, 24, rue Lhomond, 75231 Paris Cedex 05, France

Tel: +1 609 227 3952
email: regnault@princeton.edu

Parafermionic chains are the simplest generalizations of the Kitaev chain to a family of Z_N -symmetric Hamiltonians. Parafermions realize topological order and they are natural extensions of Majorana fermions. In the seminal work by P. Fendley[1], a strict notion of topological order for these systems is developed. Instead, we propose two essential properties of a topologically-ordered phase on an open chain: (i) the groundstates are mutually indistinguishable by local, symmetric probes, and (ii) a generalized notion of zero edge modes which cyclically permutes the groundstates under the Z_N generator. These properties are shown to be topologically robust, and applicable to a much wider family of topologically-ordered Hamiltonians than has been previously considered. Through a bulk-edge correspondence, we identify a many-body signature of a topologically-ordered phase on a closed chain, which offers a reliable numerical and analytical method of detection.

1. P. Fendley, J. Stat. Mech., P11020 (2012).

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Interplay between Kondo and Majorana Interactions in Quantum Dots

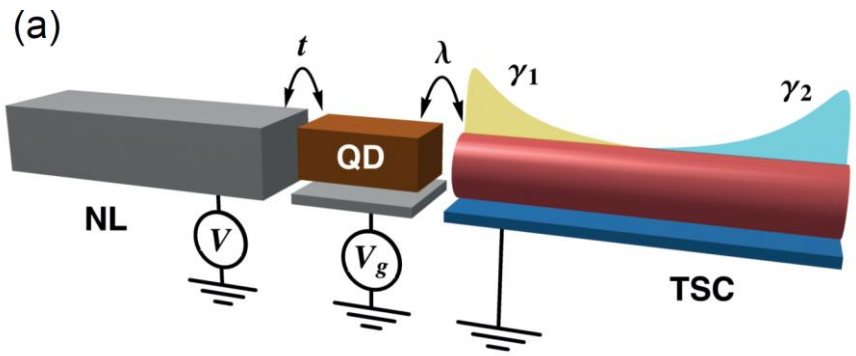
Meng Cheng, Michael Becker, Bela Bauer, and Roman M. Lutchyn

Microsoft Research, Station Q,
CNSI Bldg., office 2239,
University of California,
Santa Barbara, CA 93106, USA

Tel: +1 805 893 8853 Fax: +1 425 708 1426
email: rolutchy@microsoft.com

We study the properties of a quantum dot coupled to a one-dimensional topological superconductor and a normal lead and discuss the interplay between Kondo and Majorana-induced couplings in quantum dot. The latter appears due to the presence of Majorana zero-energy modes localized at the ends of the one-dimensional superconductor. We investigate the phase diagram of the system as a function of Kondo and Majorana interactions using a renormalization-group analysis, a slave-boson mean-field theory and numerical simulations using the density-matrix renormalization group method. We show that, in addition to the well-known Kondo fixed point, the system may flow to a new fixed point controlled by the Majorana-induced coupling which is characterized by non-trivial correlations between a localized spin on the dot and the fermion parity of the topological superconductor and normal lead. We compute several measurable quantities such as differential tunneling conductance and impurity spin susceptibility which highlight some peculiar features characteristic to the Majorana fixed point.

1. M. Cheng, M. Becker, B. Bauer, R. M. Lutchyn, Interplay between Kondo and Majorana interactions in quantum dots, arXiv:1308.4156 (2013), to appear in PRX



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Observation of Majorana Fermions in a New Platform

B. Andrei Bernevig

Department of Physics
Princeton University
Princeton, NJ 08544, USA

email: bernevig@princeton.edu

Majorana Fermions have been proposed to exist at the boundaries of one-dimensional topological superconductors. Glimpses of these particles have been seen in nanowires with spin-orbit coupling proximitized by s-wave superconductors, but their observation as edge modes of a topological superconductor has not been yet proved. We propose a new theoretical platform in which Majorana fermions can be obtained. This platform consists of magnetic atomic chains placed on top of a surface of a heavy element superconductor. We theoretically show that topologically nontrivial states are ubiquitous in this system. We then present experimental measurements which show the existence of Majorana end states in this new system.

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Gapped Symmetric Surfaces for Topological Insulators and Superconductors

Lukasz Fidkowski, F. Burnell, X. Chen, and A. Vishwanath

Department of Physics and Astronomy
Stony Brook University
Stony Brook, NY 11794-3800, USA

Tel: +1 650 796 5649 Fax: +1 631 632 8176
email: lukasz.fidkowski@stonybrook.edu

In addition to the usual 2D fractional quantum Hall realization of Majorana fermions, these exotic quasiparticles have also been predicted to exist in hc/2e fluxes at a superconducting surface of a topological insulator. Here we show that interactions which gap out the surface Dirac cone without breaking the U(1) charge conservation or time reversal symmetries necessarily lead to an exotic, topologically ordered surface state with deconfined Majorana excitations [1]. This topological order cannot be realized in a purely 2D system with the same symmetries. We also discuss a similar construction for 3D topological superconductors (class DIII) [2], which at mean field are characterized by an integer invariant n; for example, the B-phase of He^3 is thought to correspond to n=1. The exotic nature of the resulting non-abelian surface state for odd n is reflected in its chiral central charge of ¼ modulo ½; in particular this means that surface pi flux vortices host *half* of a Majorana excitation. As a consequence of our construction, we also show that this integer classification is reduced modulo 16 in the presence of interactions.

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Symmetry Protection beyond Band Theory: Constructing Bosonic Symmetry-Protected Phases in 3D

F. J. Burnell, Xie Chen, Lukasz Fidkowski, and Ashvin Vishwanath

Department of physics and astronomy, University of Minnesota
116 Church St SE, Minneapolis, MN 55455, USA

Tel: +1 612 624 0319
email: fburnell@umn.edu

Topological insulators were first understood via their topologically nontrivial band structures. Even in the presence of strong interactions, however, their distinctive gapless surface states distinguish them from ordinary insulators. This allows for the identification of analogues of topological insulators and superconductors in (strongly interacting) bosonic systems. I will discuss one such phase, the bosonic topological superconductor, and present a model Hamiltonian that realizes it.

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Electrostatic Control of Spin Polarization in a Quantum Hall Ferromagnet: A New Platform to Realize non-Abelian Excitations

A. Kazakov[1], V. Kolkovsky[2], Z. Adamus[2], T. Wojtowicz[2], and Leonid Rokhinson[1]

[1] Department of Physics, Purdue University, West Lafayette, USA

[2] Polish Academy of Sciences, Warsaw, Poland

Tel: +1 765 494 3014 Fax: +1 765 494 0706
email: leonid@purdue.edu

We develop new heterostructures where a sign of the effective g-factor of electrons in a 2D gas can be changed by electrostatic gating at high magnetic fields. This unconventional behavior is achieved in high mobility CdTe quantum wells with engineered placement of Mn atoms. In a quantum Hall regime such tunability allows one to form domains of quantum Hall ferromagnets, with domain walls consist of counter-propagating edge states of opposite polarization. Apart from interesting spintronics applications, these re-configurable domain walls can form a new platform where Majorana fermions, parafermions, Fibonacci fermions and generalized topological defects can be created, braided, manipulated and fused in a controllable fashion. I will discuss our first results where electrostatic control of the 2D gas polarization in a QHE regime is demonstrated.

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The Bulk-Edge Correspondence in Abelian Fractional Quantum Hall States

Jennifer Cano, Meng Cheng, Michael Mulligan, Chetan Nayak, Eugeniu Plamadeala, and Jon Yard

Department of Physics, Stanford University, Stanford, CA 93105, USA

Tel: +1 650 305 9599
email: michael.c.mulligan@gmail.com

It is commonly assumed that a given bulk quantum Hall state and its low energy edge excitations are in one-to-one correspondence. I will explain, contrary to this conventional wisdom, how a given bulk state may host multiple, distinct edge phases. I will describe a few surprising examples of this phenomenon that, in the simplest cases, occur at both integer, $\nu = 8$ and 12, and fractional filling fractions, $\nu = 8/7$, 12/11, 8/15, 16/5, and discuss experimentally-testable consequences. I will conclude by providing a general criterion for the existence of multiple distinct chiral edge phases for the same bulk phase.

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2. J. Cano, M. Cheng, M. Mulligan, C. Nayak, E. Plamadeala, and J. Yard. “Bulk-Edge Correspondence in 2+1-Dimensional Abelian Topological Phases.” Phys. Rev. B 89, 115116 (2014), arXiv: 1310.5708 [cond-mat].

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From Transport in Topological Insulators to the Hybrid Structures: In the Search of Majorana Fermions

Ewelina M. Hankiewicz[1], Laurens W. Molenkamp[2], and Shoucheng Zhang[3]

[1] Institute for Theoretical Physics, Wurzburg University,
Am Hubland, Wuerzburg 97074, Germany

[2] Experimental Physics (EP3), Wurzburg University,
Am Hubland, Wuerzburg 97074, Germany

[3] Department of Physics, Stanford University,
Stanford, CA 94305-4060, USA

Tel. +49 931 31 84998, Fax: +49 931 318 5141

email: Hankiewicz@physik.uni-wuerzburg.de

Topological insulators (TIs) have a bulk energy gap that separates the highest occupied band from the lowest unoccupied band, while gapless electronic states that are protected by time reversal symmetry live at the edge [1].

I will focus on transport properties of topological insulators when the Fermi energy probes the helical edge states or gapless surface states where a spin follows a momentum. In particular I will discuss how the helical edge states merge to the metal and how they can be detected through the electrical response [2].

Concerning hybrid structures, I will consider superconductor(S)/surface state of topological insulator (TI)/superconductor (S) Josephson junctions, where the S regime describes the surface state of the TI in the proximity with the s-wave superconductor. The novelty of such S/TI/S junctions originates from the electron spin helicity (locking of the momentum and the spin for a surface of TIs) which leads to both the s-wave singlet and the p-wave triplet pairing on the surface underneath the superconductor [1]. Existence of these two superconducting channels leads to novel features in transport. In particular, we show that the topological Andreev bound state (ABS) (the state of hybridized two helical Majorana fermions)) occurs for the normal incidence where ABS is protected against backscattering [3]. This topological helical ABS is characterized by the novel effect which we dubbed superconducting Klein tunneling (tunneling of the helical ABS with the transmission one through the normal regime independent of the barrier strength). The experimental setups to observe the topological helical ABS state will be proposed.

This research is supported by by the Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, under contract DE-AC02-76SF00515, DFG grant HA 5893/4-1 within SPP 1666 and DFG-JST joint research project 'Topological Electronics'

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2. C. Brüne, A. Roth, H. Buhmann, E. M. Hankiewicz, L. W. Molenkamp, J. Maciejko, X.-L. Qi and S.-C. Zhang, Nature Physics 8, 486 (2012).
3. G. Tkachov and E. M.Hankiewicz, Phys. Rev. B 88, 075401 (2013).

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Weber Blockade in Superconducting Nanowires

Tyler Morgan-Wall, Benjamin Leith, Nikolaus Hartman, Atikur Rahman, and Nina Markovic

Department of Physics and Astronomy, Johns Hopkins University,
3400 N Charles Street, Baltimore, Maryland 21218, USA

Tel: +1 410 516 6422 Fax: +1 410 516 7239
email: nina@pha.jhu.edu

Superconducting nanowires are essential components of many quantum devices, from single photon detectors, to flux qubits and Majorana detection and manipulation schemes. With this in mind, we have developed a method for fabrication of ultranarrow nanowires with controlled normal resistance and consistent superconducting properties [1]. In magnetic field, the superconductivity in wider nanowires is affected by vortices, topological excitations that can be viewed as basic degrees of freedom of the system. We show that a short superconducting nanowire can behave as a quantum dot for vortices. In the range of magnetic fields in which vortices can enter the nanowire in a single row, we find regular oscillations of the critical current as a function of magnetic field, with each oscillation corresponding to the addition of a single vortex to the nanowire [2]. A charge-vortex dual of the Coulomb-blockaded quantum dot for electrons, the nanowire shows diamond-shaped regions of zero resistance as a function of current and magnetic field, in which the number of vortices is fixed. In addition to showing that macroscopic objects such as vortices can behave as fundamental particles, the demonstrated fine control over critical currents and vortex configurations can be utilized in novel quantum devices.

This research is supported by the NSF Grant No. DMR-1106167

1. T. Morgan-Wall, H. J. Hughes, N. Hartman, T. M. McQueen and N. Markovic, Appl. Phys. Lett. 104, 173101 (2014).
2. T. Morgan-Wall, B. Leith, N. Hartman, A. Rahman, and N. Markovic, arXiv:1406.6802.

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Counting Statistics of Single-Electron Thermal Noise

Katsuhiko Nishiguchi[1], Yukinori Ono[2], and Akira Fujiwara[1]

[1] NTT Basic Research Laboratories,

[2] Graduate School of Science and Engineering, University of Toyama

3-1 Morinosato Wakamiya, Atsugi, Kanagawa 243-0198, Japan

Tel: +81 46 240 2477 Fax: +81 46 240 4317
email: nishiguchi.katsuhiko@lab.ntt.co.jp

Noises in electric devices always degrade their performance. In particular, since shrinkage of a transistor reduces the number of electrons in the transistor, degradation of device performance caused by noise has become more serious. Therefore, although the history of research about the noise is long, the investigation of noise is still of great interest and recently has been extended to single-electron resolution.

In this work, thermal noise, one of the most well-known, fundamental, and unavoidable types of noise in all electronic devices, is monitored in real time with single-electron resolution by using a nanometer-scale transistor at room temperature. It is confirmed that single-electron thermal noise perfectly follows all the aspects predicted by the statistical mechanics, which include the occupation probability, the law of equipartition, a detailed balance, and the law of kT/C. In addition, the real-time monitoring of the electron motion silhouettes anisotropic single-electron motion in transistor, its power spectrum density, and shot-noise-like characteristics buried in the thermal noise. These results will play an important role in future electronic devices as well as academic research in areas such as the counting statistics of thermal noise.

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Pattern Classification by Memristive Crossbar Array

Mirko Prezioso, Farnood Merrikh-Bayat, Brian Hoskins, Gina Adam, and Dmitri Strukov

Electrical and Computer Engineering Department,
University of California at Santa Barbara, Santa Barbara,
CA 93106, USA

Tel: +1 805 893 2095 Fax: +1 805 893 3262
email: mprezioso@ece.ucsb.edu

This abstract is not printed due to the authors' request.

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Singe-Metal Nanoscale Thermocouples

Gergo P. Szakmany, Alexei O. Orlov, Gary H. Bernstein, and Wolfgang Porod

Center for Nano Science and Technology
University of Notre Dame, IN 46556, USA

Tel: +1 574 631 6376 Fax: +1 574 631 4393
email: porod@nd.edu

We study the generation of thermoelectricity by nanoscale thermocouples formed from a single layer of metal with cross-sectional discontinuity. Typically, a thermocouple is formed from a second metal inserted between two sections of a first metal. Here, we investigate the behavior of TCs formed not of two metals but rather nanowires of the same metal of two cross-sectional areas. Mono-metallic thermocouples (TC) were constructed from a lithographically defined nanowire having one abrupt variation in width along its length, and tested at room temperature; these structures exploit a change in Seebeck coefficient that is present at these size scales. To investigate the thermoelectric properties of such “shape-engineered” thermocouples, nanoscale heaters were employed to control local temperatures. Temperature profiles at the hot and cold junctions of the TCs were determined both by simulations and experiments. Results demonstrate that the magnitude of the open-circuit voltage, and hence the relative Seebeck coefficient, is a function of the parameters of the variations in the segment widths. The fabrication complexity of such shape-engineered mono-metallic nanowire TCs is greatly reduced compared to that of conventional bi-metallic TCs, and could be mass-produced using simpler manufacturing techniques.

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Quantum Control using Trapped Ions

Michael J. Biercuk

ARC Centre for Engineered Quantum Systems, School of Physics
The University of Sydney, NSW 2006, Australia

Tel: +61 2 9036 5301
email: michael.biercuk@sydney.edu.au

Tremendous research activity worldwide has focused on attempting to harness the quantum physical phenomena for new applications in metrology, computation, and communications - a push to develop engineered quantum systems. Underlying any such capability is the need to exert control over a chosen quantum system in order to coax it into performing useful tasks. In this talk we introduce the problem of control engineering in these systems and show how advances in control may help to address longstanding challenges in the research community. We focus on new frequency-domain techniques allowing the precise prediction of quantum dynamics in the presence of time-dependent control and environments, accounting for the possible presence of non-commutative Hamiltonian terms. This is a key requirement for deploying quantum systems in demanding applications from quantum computation to precision metrology. Through a series of experiments using trapped ions we validate this technique and demonstrate its utility for decoherence suppression and elucidating subtleties in the physics underlying the time-evolution of quantum systems. We highlight the role of these control techniques for applications in studies of quantum many-body phenomena through the realization of *programmable* quantum simulation, showing the versatility of the trapped-ion platform and a path towards large-scale quantum technologies.

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2. D.Hayes, S.T. Flammia, M.J. Biercuk, “Programmable quantum simulation by dynamic Hamiltonian engineering” *New J. Phys.* 16, 083027 (2014).

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Nanowire Quantum Dots in a Superconducting Microwave Cavity

Russell S. Deacon, Rui Wang, Tomohiro Yamaguchi, Yuji Yamazaki, Kenji Wada, and Koji Ishibashi

Advanced Device Laboratory and Center for Emergent Matter Science (CEMS), RIKEN
2-1, Hirosawa, Wako, Saitama 351-0198, Japan

Tel: +81-48-467-9367 Fax: +81-48-462-4659
email: kishiba@riken.jp

A single individual spin can be a good candidate to store quantum information. The coupling of the spin with a microwave circuit cavity may open a new possibility for the quantum processing devices and architectures. To realize electrical control of the spin with the electric field, we have been working on InSb or Ge/Si core/shell nanowire quantum dots which have a strong spin-orbit interaction. In this report, we will present preliminary results on the fabrication of InSb coupled quantum dots in a superconducting microwave cavity and microwave resonance measurements in dilution refrigerator temperatures when the coupled quantum dots are formed.

A InSb NW was located between the signal and grand lines, and the finger gates were fabricated underneath the NW with a HfO insulating layer in between to form the coupled quantum dots. DC transport measurements and the microwave transmission measurements were performed simultaneously, and we could see the honeycomb-like pattern unique to the double dots in both DC and MW phase measurements. An interesting feature was that a few-electron regime was measured in the microwave measurement, while it was impossible with the DC measurement because the current was too small to detect. The resonant frequencies were different, depending on the situations where an electron is localized in one dot, or it can move back and forth between the two dots (on the charge degeneracy line). We do not understand the mechanism of the frequency shift, but presume it is due to the quantum mechanical coupling of the electric charge dipole and the cavity photons.

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Addressable Control of Three Spin Qubits in Semiconductor Triple Quantum Dot

Takashi Nakajima[1,2], Matthieu R. Delbecq[1,2], Tomohiro Otsuka[1,2], Shinichi Amaha[1], Jun Yoneda[1,2], Akito Noiri[2], Arne Ludwig[3], Andreas D. Wieck[3], and Seigo Tarucha[1,2]

[1] Center for Emergent Matter Science, RIKEN
2-1 Hirosawa, Wako-shi, Saitama 351-0198, Japan

[2] Department of Applied Physics, University of Tokyo
3-8-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan

[3] Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum
Universitätsstraße 150, 44780 Bochum, Germany

Tel: +81-48-467-9470 Fax: +81-62-4672
email: nakajima.physics@icloud.com

Electron spin in semiconductor quantum dots (QDs) is promising building block of quantum computers, not least for potential scalability [1]. By employing magnetic field gradient induced by micro-magnet (MM) deposited on top of QDs[2], single-spin manipulation with fidelity up to 97% was realized recently[3]. It is, however, not straightforward to scale up of the system to three or more qubits because conventional DC transport measurement in the spin blockade regime is no longer applicable.

We recently realized individual control of single spins in a laterally coupled triple QD defined by gate electrodes. Spin states were initialized and readout by pump and probe technique with detuning pulse. Each spin state was manipulated by electron spin resonance and addressed by different resonance frequency due to local Zeeman field induced by the MM. We will discuss key properties for the application of this system to three-qubit quantum algorithms.

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Interlayer Charge Transfer and Spin State Transitions in a Triple-layered Quantum Hall System

Shinichi Amaha[1,*], Tsuyoshi Hatano[2], Takashi Nakajima[1], Kimitoshi Kono[1], and Seigo Tarucha[1, 3]

[1] Center for Emergent Matter Science, RIKEN
2-1 Hirosawa, Wako-shi, Saitama 351-0198, Japan

[2] Department of Physics, School of Science, Tohoku University,
6-3 Aramaki aza Aoba, Aoba-ku Sendai, Miyagi 980-8578, Japan

[3] Department of Applied Physics, University of Tokyo
3-8-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan

[*]Tel: +81-48-467-9470 Fax: +81-48-462-4672
email: s-amaha@riken.jp

Bi-layer two-dimensional electron systems have been eagerly studied due to the intriguing phenomena associated with interlayer Coulomb interaction and coherence - e.g. the tunnelling in two layers at Landau filling factor ν=1 [1], and the spin canted phase in ν=2 [2]. From the aspect of enhanced freedom in layer degree, tri-layer quantum Hall systems (TQSs) are attracting more interests [3]. However, the experimental reports on the TQSs have been limited due to the difficulty of material fabrication [4].

We investigate charge and spin state transitions in TQS embedded in triple quantum well as a function of front, back gate voltages (V_{GF}, V_{GB}) and external magnetic field. By sweeping V_{GF} and V_{GB}, the offsets between the wells can be modified, and concurrently the charge state in each well is also modulated. By examining the conductance, we assigned the charge transfer from single, double to triple quantum wells. We also observed spin state transitions in total filling factor ν=3 and 4, which can be pictorially understood by the model where electrons are confined in the single particle levels with the ferromagnetic exchange interactions. Our investigations is useful to explore the novel physics and new quasi-particle excitations in the TQSs.

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Topological Matter as New forms of 2D Electron Systems: Fundamental Physics with Potential for Application

M. Zahid Hasan

Department of Physics, Princeton University, Princeton, NJ 08544, USA

Tel: +1 609 258 3044 Fax: +1 609 258 1006
email: mzhasan@princeton.edu

In this talk, I briefly review the basic concepts defining topological matter and the key experimental results that revealed and established their novel character. I then report our recent results on topological quantum phase transition leading to the realization of 3D Graphene, topological Dirac semimetals (TDSM), topological Crystalline Insulators (TCI), topological Kondo Insulators (TKI) and topological superconductors (TSC) [1-6]. Some recent results on thin-film topological superconductors as a robust platform for Majorana Fermions would be presented. These new phases of electronic matter collectively reveal the emergence of a topological revolution in condensed matter physics with potential for application.

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Aharonov-Bohm Oscillations in a Quasi-Ballistic 3D Topological Insulator Nanowire

S. Cho, B. Dellabetta, A. Yang, J. Schneeloch, Z. J. Xu, G. Gu, M.J. Gilbert, and N. Mason

Department of Physics and Frederick Seitz Materials Research Laboratory
104 South Goodwin Avenue, University of Illinois, Urbana, Illinois 61801, USA

Tel: +1 217 244 9114 Fax: +1 217 244 8544
email: nadya@illinois.edu

In three-dimensional topological insulator (3D TI) nanowires, transport occurs via gapless surface states where the spin is fixed perpendicular to the momentum. Evidence of surface state transport has previously been demonstrated via Aharonov-Bohm (AB) oscillations in magnetoresistance, which occur due to the coherent propagation of electrons around the circumference of the nanowire. However, signatures of the topological nature of the surface state (i.e., a Berry's phase) have been missing. By fabricating quasi-ballistic 3D TI nanowire devices gate tunable through the Dirac point, we have been able to demonstrate the salient features of AB oscillations not seen in other non-topological nanowire systems. In particular, we observe alternations of conductance maxima and minima with gate voltage, and conductance minima near $\Phi/\Phi_0 = 0$ with corresponding maxima of ~ e^2/h near $\Phi/\Phi_0 = 0.5$, which is consistent with the existence of a low-energy topological mode. The observation of this mode is a necessary step toward utilizing topological properties at the nanoscale in post-CMOS applications, for example, in topological quantum computing devices or as efficient replacements for metallic interconnects in information processing architectures.

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Electromagnetic Response Properties and Signatures of 2D and 3D Topological Semi-Metals

Srinidhi T. Ramamurthy and Taylor L. Hughes

Institute for Condensed Matter Theory, University of Illinois at Urbana-Champaign
1101 W Green St. Urbana, IL 61801, USA

Tel: +1 650 704 5898 Fax: +1 217 244 7704
email: hughest@illinois.edu

The rise of topological insulator materials over the past decade has generated an outpouring of theoretical and experimental work. These insulating systems have some remarkable properties, and transitioning them to technological applications has been an exciting challenge. A related set of materials is the class of topological semi-metals, which are not insulating in the bulk but instead have point or line-like Fermi surfaces. Some examples of these states are the 2D and 3D Dirac semi-metals (e.g., graphene) and the 3D Weyl semi-metal. These materials have interesting surface properties and quasi-topological electromagnetic response properties arising from the bulk states. We present theory and simulations that fully describes these bulk response properties for point-node and line-node semi-metals. We show how these properties are tied to the geometrical properties of the Fermi-surfaces and how point-group and discrete symmetries can act to stabilize these metallic phases.

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Proximity-Induced Phenomena in Hetero-Structures Involving Topological (Crystalline) Insulators

Turgut Yilmaz, Ivo Pletikosic, Andrew Weber, Jurek Sadowski, Genda Gu, Boris Sinkovic, and Tonica Valla

Brookhaven National Laboratory,
Brookhaven Ave. 734, Upton, NY 11973, USA

Tel: +1 631 344 3530 Fax: +1 631 344 2739
email: valla@bnl.gov

Topological insulators (TI) and topological crystalline insulators (TCI) are predicted to show a variety of very unusual phenomena when interfaced with magnetic and superconducting materials, ranging from induced magnetic monopoles, quantum anomalous Hall effect, Majorana and Weyl fermions, etc. Some of these exotic phenomena might be used for spintronics applications, magnetic recording and quantum computing, but problems with materials and very stringent constraints on physical parameters render the wide-spread applications extremely difficult. Therefore, both the materials synthesis and the physical parameters constraints have to be explored and optimized. Here, we present the angle and spin resolved photoemission spectroscopy studies of various *in-situ* grown TI and TCI hetero-structures involving interfaces with magnetic and superconducting materials in a wide range of thicknesses and compositions of building blocks. We discuss the observed features in the low-energy electronic spectra and relate them to the relevant macroscopic properties.

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Synthetic Topological Qubits in Conventional Bilayer Quantum Hall Systems

Maissam Barkeshli and Xiao-Liang Qi

Microsoft Station Q,
Elings Hall Rm. 2243, University of California
Santa Barbara, CA 93106, USA

Tel: +1 408 621 2556
email: mbarkeshli@gmail.com

The idea of topological quantum computation is to build powerful and robust quantum computers with certain macroscopic quantum states of matter called topologically ordered states. These systems have degenerate ground states that can be used as robust “topological qubits” to store and process quantum information. Here, we propose a new experimental setup which can realize topological qubits in a simple bilayer fractional quantum Hall (FQH) system with proper electric gate configurations. Our proposal is accessible with current experimental techniques, involves well-established topological states, and moreover can realize a large class of topological qubits, generalizing the Majorana zero modes studied in the recent literature to more computationally powerful possibilities. We propose several experiments to detect the existence and non-local topological properties of the topological qubits.

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Topological Insulators in Electronic and Spintronic Applications

Leonard F. Register, Urmimala Roy, Rik Dey, Tanmoy Primanik, Jiwon Chang, and Sanjay K. Banerjee

The University of Texas at Austin, Department of Electrical and Computer Engineering, and Microelectronics Research Center, USA

Tel: +1 512 567 3748
email: register@utexas.edu

Topological insulators (TIs) have novel properties that may be exploitable for both conventional and novel device applications. While topological insulators are three-dimensional (3D) materials, their electronic surface states are quasi-two dimensional (2D), with a gapless band-structure featuring Dirac cones much like graphene, although located at the Brillouin zone center, and fast carriers of perhaps half the velocity of those in graphene. However, band-gaps are created in the surface states of thin TIs, potentially making them suitable for conventional CMOS applications. Perhaps the most intriguing features of TIs for device applications is the spin-helical locking of the surface states, which could make them a natural for spintronic device applications, providing a natural tool for translating between charge and spin transport. Thus, TIs could provide perhaps novel memory and switching possibilities, such as their own unique version of a giant spin Hall effect for spin transfer torque, while also allowing integration with conventional devices implemented in TIs. However, there are also less than ideal characteristics of TI for such applications as well. In this presentation, we illustrate a select few of the possibilities, associated challenges, and perhaps work-a-rounds based on our past and current research.

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Using Monolayer-Tin-based Topological Insulators for Transistor Applications

William Vandenberghe and Massimo Fischetti

Dept. of Materials Science and Engineering, The University of Texas at Dallas
800 West Campbell Rd, RL10, Richardson, TX 75080, USA

Tel: +1 214 600 4900 Fax: +1 972 883 5725
email: wxv101020@utdallas.edu

Monolayers of tin (stannanane) functionalized with halogens have been shown to be topological insulators. Using density functional theory (DFT) we study the electronic properties and room-temperature transport of nanoribbons of iodine-functionalized stannanane showing that the overlap integral between the wavefunctions associated to edge-states at opposite ends of the ribbons decreases with increasing width of the ribbons. Obtaining the phonon spectra and the deformation potentials also from DFT, we calculate the conductivity of the ribbons using the Kubo-Greenwood formalism and show that their mobility is limited by inter-edge phonon backscattering. We show that wide stannanane ribbons have a mobility exceeding 10^6 cm^2/Vs. Contrary to ordinary semiconductors, two-dimensional topological insulators exhibit a high conductivity at low charge density, decreasing with increasing carrier density. Furthermore, the conductivity of iodine-functionalized stannanane ribbons can be modulated over a range of three orders of magnitude, thus rendering this material extremely interesting for classical computing applications.

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Quantum Strain Sensor with a Topological Insulator HgTe Quantum Dot

Marek Korkusinski and Pawel Hawrylak

Department of Physics,
University of Ottawa
MacDonald Hall,150 Louis Pasteur
Ottawa, Ontario, K1N 6N5, Canada

Tel: +1 613 562 5800 ext 2690

e-mail: pawel.hawrylak@uottawa.ca

We present a theory of electronic properties of HgTe quantum dot and propose a strain sensor based on a strain-driven transition from a HgTe quantum dot with inverted bandstructure and robust topologically protected quantum edge states to a normal state without edge states in the energy gap. The presence or absence of edge states leads to large on/off ratio of conductivity across the quantum dot, tunable by adjusting the number of conduction channels in the source-drain voltage window.

The electronic properties of a HgTe quantum dot as a function of size and applied strain are described using eight-band k·p Luttinger and Bir-Pikus Hamiltonians, with surface states identified with chirality of Luttinger spinors and obtained through extensive numerical diagonalization of the Hamiltonian [1].

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Tuning of the Transition Temperature to the Charge-Density-Wave State in $TaSe_2$ and $TiSe_2$ Thin Films

R. Samnakay, C. Jiang, J. Renteria and A.A. Balandin

Department of Electrical and Computer Engineering and Materials Science and Engineering Program, Bourns College of Engineering, University of California – Riverside, CA 92521 USA

Tel: +1 951 827 2351 Fax: +1 951 827 2425
email: balandin@ee.ucr.edu

A charge density wave (CDW) is a symmetry-reducing ground state most commonly found in layered materials. The appearance of a CDW state results from the Peierls instability [1]. Below the transition temperature T_C, the lattice of atoms undergoes a periodic distortion and the electrons condense into a ground state with a periodic modulation of the charge density leading to an energy gap at the Fermi surface. The CDW collective quantum states were proposed for information processing [2-3]. In this talk we show that T_C can be tuned in thin films of CDW materials by changing their thickness. We used mechanical exfoliation of $TiSe_2$ and $TaSe_2$ crystals to prepare a set of films. The temperature T_C to the CDW state was determined via modification of Raman spectra of the films. It was established that T_C of $TiSe_2$ can increase from its bulk value of 200 K to ~240 K as the thickness of the films reduces to the nanometer range. The 1T-$TaSe_2$ polytype is in CDW phase below T_C of 473 K. It was established that T_C decreases from its bulk value to ~413 K as the thickness of the 1T-$TaSe_2$ films is reduced from 150 nm to around 35 nm. The experimentally observed trends are in agreement with theoretical calculations. The obtained results are important for the proposed applications of such materials in the collective-state information processing.

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Measurement of High Exciton Binding Energy in the Monolayer Transition-Metal Dichalcogenides WS_2 and WSe_2

Aubrey T. Hanbicki[1], Marc Currie[1], George Kioseoglou[2], Adam L. Friedman[1], and Berend T. Jonker[1]
[1] Naval Research Laboratory, 4555 Overlook Ave. SW, Washington, DC 20375 USA
[2] University of Crete, Heraklion Crete, 71003, Greece

Tel: +1 202 404 8015 Fax: +1 202 404 4637
email: berry.jonker@nrl.navy.mil

Monolayer transition-metal dichalcogenides are direct gap semiconductors with great promise for optoelectronic devices. Although spatial correlation of electrons and holes plays a key role, there is little experimental information on such fundamental properties as exciton binding energies and band gaps. We report here an experimental determination of exciton excited states and binding energies for monolayer WS_2 and WSe_2. We observe peaks in the optical reflectivity/absorption spectra corresponding to the ground- and excited-state excitons (*1s* and *2s* states). From these features, we determine lower bounds free of any model assumptions for the exciton binding energies as E_{2s}^{A} - E_{1s}^{A} of 0.83 eV and 0.79 eV for WS_2 and WSe_2, respectively, and for the corresponding band gaps E_g ~ E_{2s}^{A} of 2.90 and 2.53 eV at 4K. These remarkably high exciton binding energies imply that excitonic behavior dominates to room temperature and above, and we are indeed able to follow the evolution of these features to 300K. Because the binding energies are large, the true band gap is substantially higher than the dominant spectral feature commonly observed with photoluminescence. This information is critical for emerging applications, and provides new insight into these novel monolayer semiconductors.

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Theory of Dual-Probe Measurements of Large Nanostructures on Two-Dimensional Materials

Mikkel Settnes, Stephen R. Power, Dirch H. Pedersen, and Antti-Pekka Jauho

Center for Nanostructured Graphene (CNG), Department of Micro and Nanotechnology, Technical University of Denmark, 2820 Kongens Lyngby, Denmark

Tel: + 45 4525 6335 Fax: +45 4588 7762
email: Antti-Pekka.Jauho@nanotech.dtu.dk

Dual-probe measurements on two-dimensional systems have recently been shown to yield a wealth of microscopic information about the scattering processes occurring in these structures, in particular if the probe separation is smaller than the dephasing length [1,2]. These two papers focused on subnanometer structures, such as defects or adatoms, and here we report a generalization to much larger structures with dimensions of tens of nanometers. Standard approaches would result in a prohibitive numerical cost, and we have developed a novel method for treating the boundary conditions: the self-energies which describe the device-to-lead coupling are generalized to a “square-self-energy”, which allows a fast treatment of large area samples. As an example, we consider nanoblisters on graphene [3], and show that the electronic transport properties display a rich phenomenology, which can be interpreted in terms of the pseudomagnetic field associated with the finite curvature of the blister. Computed bond currents show vortices, and suggest that new functionalities can be achieved by varying the size of the blister by controlling its pressure.

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Evaluation of Heterojunction Nanowire Transistor Options for 7nm CMOS

Asen Asenov, Craig Riddet, and Ewan Towie

Affiliation The University of Glasgow and Gold Standar Simulations
Address Rankine Building, Oakfield Avenue, Glasgow G12 8LT, United Kingdom

Tel: +44 141 330 4790 Fax:
Email: Asen.Asenov@Glasgow.ac.uk

The development of the next generation CMOS technologies require the introduction of novel transistor architecture and novel channel and gate dielectric materials. After the introduction of FDSOI at 28nm CMOS by ST Microelectronics and the introduction of FinFETs at 22 nm by Intel Nanowire transistors are on the table for 7nm and beyond CMOS technologies. This will be in combination with the introduction of novel channel materials to enhance the transistors performance and corresponding novel high-k dielectric stacks. Simulation of such devices is a great challenge due to strong quantum mechanical effects including 1D non-equilibrium quasi-ballistic transport. We will report on the development of new simulation tools that handle the above challenges and allow the predictive simulations and screening of the technology options at 7nm CMOS. Apart from quantum-corrected Monte Carlo simulation techniques we will discuss a hybridisation between NEGF simulation technology and 1D multi-subban Monte Carlo simulation techniques. The interfacing of the above simulation techniques to first principle electronic structure calculations will be also discussed. We will provide examples including nanowire transistors with different channel cross sections and channel materials and will draw conclusions about the advantages and disadvantages of the different approaches.

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How Much Time does FET Scaling have left?

Denis Mamaluy, Xujiao Gao, and Brian Tierney

Sandia National Laboratories
P.O. Box 5800, MS 1322
Albuquerque, NM 87185-1322, USA

Tel: +1 505 844 2054, Fax: +1 505 284 2518
email: mamaluy@sandia.gov

Utilizing our fully 3D charge self-consistent quantum transport simulator, CBR3D, we computed the electrical characteristics and switching energy, $C_gV_g^2$, for a number of representative FinFET/MuGFET devices, which were optimized (geometry, doping profiles) to satisfy ITRS specifications [1] for high-performance devices at 6-, 5-, and 4nm gate lengths. We have found that the industry is approaching the fundamental down-scaling limit for CMOS technology and other FETs. Specifically, we predict that at room temperatures FETs, *irrespectively of their channel material*, will start experiencing unacceptable level of thermally induced errors around 5-nm gate lengths. This effectively means the end of Moore's law for FETs (including TFETs), which would happen, according to the current ITRS projections, in less than 15 years from now. We will discuss the industry possibilities after the thermal fluctuation limit is reached and a particular prospect of *overcoming* this limit with SET-logic devices and the consequent downscaling of SET-based switches to sub-5nm dimensions for room temperature operation.

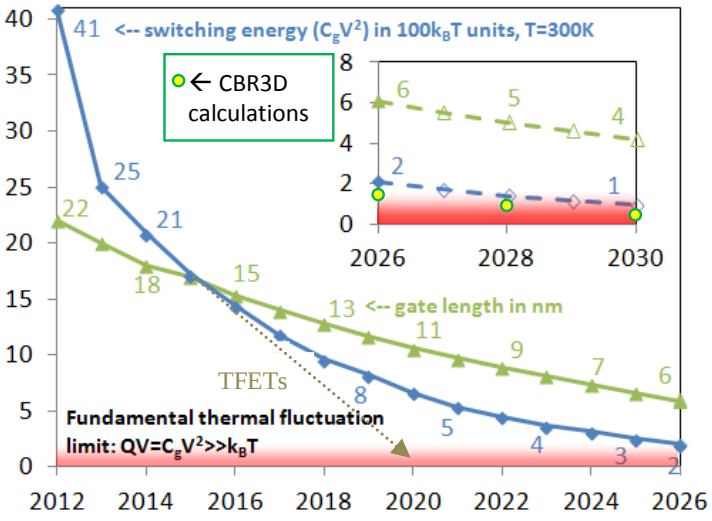

Figure 1. ITRS gate length projection (green) for high performance MuGFET devices and associated calculated switching energy (blue). Inset shows corresponding CBR3D switching energy calculations for optimized devices.

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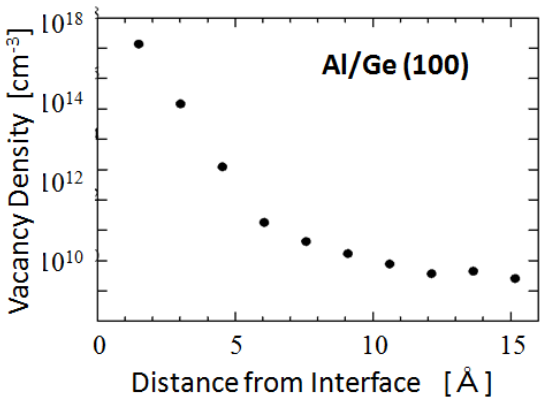
Why Defect Density Remarkably Increases at Metal/Ge Interfaces: Control of Metal-induced Gap States

Takashi Nakayama, Shogo Sasaki, and Tomoki Hiramatsu

Department of Physics, Chiba University
Yayoi 1-33, Inage, Chiba 263-8522, Japan

Tel: +81-43-290-2762 Fax: +81-43-290-2874
email: nakayama@physics.s.chiba-u.ac.jp

Because of high electron mobility, germanium (Ge) is again expected as a promising post-Si material for next-generation high-speed mainstream devices. Due to its small cohesive energy, however, Ge has many defects such as vacancy compared to Si, especially around metal/Ge interfaces. The defects are key elements to determine the interface properties such as Schottky barrier (SB). However, our knowledge is still limited for metal/Ge interfaces. In this work, we have studied fundamental properties of point defects around metal/Ge interfaces by the first-principles calculations, i.e., how many defects like vacancy and interstitial impurities are distributed around metal/Ge interfaces and how they change the SB. We found that the defect density remarkably increases around the interface[1] (See figure) and induces the strong SB pinning because the hybridization of defect states with the metal-induced gap states (MIGS) stabilizes the defects. The results indicate that the MIGS is important not only for determining the SB but also for inducing the defect distribution around the metal/Ge interfaces.



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Increasing the Asymmetry of Metal-Insulator-Insulator-Metal (MIIM) Tunnel Diodes through Defect Enhanced Direct Tunneling (DEDT)

John F. Conley, Jr. and Nasir Alimardani

School of Electrical Engineering and Computer Science, Oregon State University
Corvallis, OR 97330, USA

Tel: +1 541 737 9874; email: john.conley@eecs.oregonstate.edu

Thin film metal-insulator-metal (MIM) tunnel diodes are of interest for a variety of high-speed beyond-Si applications. Rectification in these devices generally based on Fowler-Nordheim tunnelling through the asymmetric electron tunnel barrier that is produced by dissimilar work function (Φ_M) metals and is limited by $\Delta\Phi_M$.[1] Performance may be improved using heterostructure insulator stacks to produce an asymmetric tunnel barrier MIIM diodes. Recently, enhanced performance in bilayer Al_2O_3/HfO_2 MIIM diodes was shown to be due to "step tunneling" (ST), a situation in which electrons under one polarity may directly tunnel through only the larger bandgap insulator instead of both insulators.[2] In this work, we show that asymmetry and V_{ON} may be further improved by pairing Al_2O_3 with Ta_2O_5, a high electron affinity (χ) insulator dominated by Frenkel-Poole emission (FPE). The observed improvements, however, are not consistent with the ST model. Instead, the enhanced performance in atomic layer deposited (ALD) Al_2O_3/HfO_2 MIIM diodes may be explained by *defect enhanced direct tunneling* (DEDT), in which electrons injected from the electrode adjacent to the Ta_2O_5 transport easily across this insulator via defect enhanced (DE) FPE before direct tunneling (DT) through the Al_2O_3. DEDT results in an effectively narrowed tunnel barrier for one polarity, as electrons traveling under the opposite polarity must tunnel through both insulators. We show that the MIIM architecture not only allows insulators dominated by FPE to be used in temperature insensitive diodes, but actually takes advantage of the defect conduction to improve performance.

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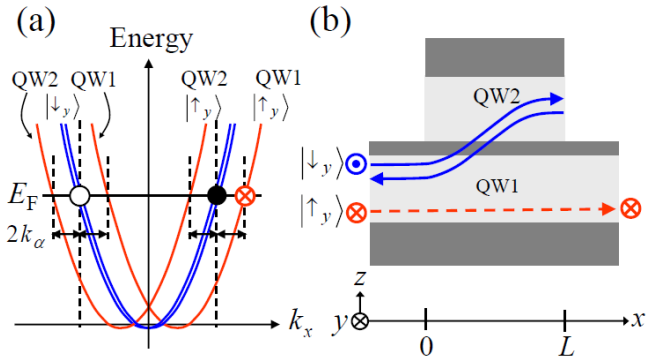
Proposal of Spin-Orbital Blockade using InGaAs/InAlAs Double Quantum Wells and Physics of Landau Level Interactions

Takaaki Koga[1], Hang Chen[1], and Satofumi Souma[2]

[1] Graduate School of Information Science and Technology, Hokkaido University, Sapporo, 060-0814, Japan
[2] Department of Electrical and Electronics Engineering, Kobe University, Kobe, 657-8501, Japan

Tel: +81-11-706-6538 Fax: +81-11-706-7802
email: koga@ist.hokudai.ac.jp

A lateral spin-blockade device that uses the Rashba effect [1,2] in the double quantum well (DQW) system is proposed. In the DQW system, the values of the Rashba spin-orbit parameter α_R can be made opposite in sign but equal in magnitude between the constituent quantum wells (QW) [3]. By tuning the size of the device and the magnitude of the externally applied in-plane magnetic field, the transmission of one spin (e.g., spin-down) component can be blocked completely, leading to a spin-polarized current [4]. Such a spin blocking effect can be brought about by wave vector matching of the spin-split Fermi surfaces between the two QWs (see the figure). We also discuss about various interactions among the Landau levels formed by the perpendicular magnetic field.



(a) Energy dispersion relation of the proposed DQW system with a tuned magnetic field **B** = (0, B_{ac}, 0).

(b) Spin dependent trajectories of electrons which are injected into QW1 from left, where the Fermi wave number matching condition is satisfied by the magnetic field **B** = (0, B_{ac}, 0).

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Graphene Spintronics: From Spin Injection to Magnetologic Gates

Igor Zutic[1], Predrag Lazic[2], Guilherme Sipahi[1,3], and Roland Kawakami[4]

[1] Department of Physics, University at Buffalo, Buffalo, NY 14260, USA
[2] Rudjer Boskovic Institute, PO Box 180, Bijenicka c. 54, 10 002 Zagreb, Croatia
[3] Instituto de Fisica de Sao Carlos, Universidade de Sao Paulo, Brazil
[4] Department of Physics, The Ohio State University, Columbus, OH 43210, USA

Tel: +1 716 645 2017 Fax: +1 716 645 2507
email: zigor@buffalo.edu

Ferromagnet/graphene (F/Gr) junctions are important building blocks to implement spin injection in spintronic devices, realizing functionalities ineffective in conventional electronics. While simple models of spin injection are very successful for macroscopic metallic junctions, they reveal many deficiencies in describing F/Gr junctions [1]. Motivated by the proposal for graphene-based magnetologic gates providing seamless integration of memory and logic [2], we formulate a computationally inexpensive first-principles model to examine the nonuniformity and bias dependence of spin injection and elucidate proximity effects using spin polarization maps [1,3]. Our results could extend the applicability of simple spin injection models to F/Gr junctions and explore novel opportunities for graphene spintronics [4].

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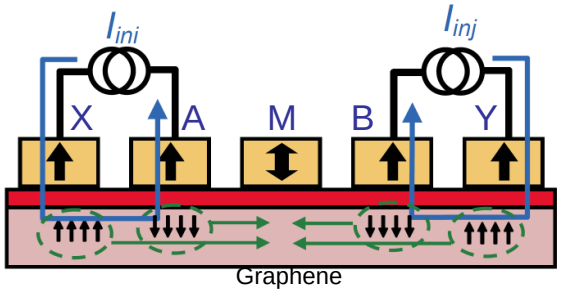

Figure 1. Magnetologic gate. The spin accumulation (small arrows) in graphene (Gr) is governed by the magnetization direction (large arrows) of the ferromagnetic (F) contact pairs of A-X and B-Y. A dynamic readout of the spin accumulation is realized by perturbing the magnetization direction of the contact M under which a pure spin current flows [2].

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Functionalized Graphene as a Spintronics Material

Jaroslav Fabian

Physics Department, University of Regensburg, 93040 Regensburg, Germany

Tel: +49-941-943-2031 Fax: +49-941-943-4382
email: Jaroslav.Fabian@ur.de

Graphene is emerging as a material for fundamental and applied spintronics. Pristine graphene has weak spin-orbit coupling and no magnetization, but functionalized with adatoms, its spin-orbit coupling is colossally enhanced [1] (this is also confirmed in experiments on the spin Hall effect), while magnetic moments appear [2]. For spintronics applications, such as graphene spin transistors, graphene has still to overcome the mysterious strong spin relaxation that has occupied researchers in this field for many years now. Only recently it was recognized that the spin relaxation in graphene is dominated by local magnetic moments which provide resonant scattering [2]. This finding shows a clear path towards long spin relaxation times, by chemically isolating the local moments. It appears that magnetic moments can come from simple adatoms such as hydrogen [2], from organic molecules covalently bonding on graphene, and even from vacancies. An open issue is the transfer of magnetization from transitional metals to graphene, which depends on the hybridization and charge transfer. Most fascinating is the perspective of graphene for controllable magnetism: our calculations show that magnetic moments can be switched off and on by an electric field across graphene bilayers. Further possibilities come from graphene on other 2d materials, such as MoS_2. Such combinations open prospects for controllable spin-orbit coupling, which can control spin current and spin relaxation. I will discuss progress and open issues in this field, from both theory and experimental point of view, and argue for graphene's perspective as a viable spintronic material.

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Surface-Induced Spin-Orbit Coupling in Metallic Films: A Theorem and an ab initio Calculation

I. V. Tokatly[1], E. E. Krasovskii[1], and G. Vignale[2]

[1] Departamento de Fisica de Materiales, Universidad del Pais Vasco UPV/EHU, 20080 San Sebastian/Donostia, Basque Country, Spain

[2] Department of Physics, University of Missouri, Columbia MO 65203, USA

Tel. +1 573 882 3670 Fax. +1 573 882 4195
email: vignaleg@missouri.edu

The broken inversion symmetry at the surface of a metallic film (or, more generally, at the interface between a metallic film and a different metallic or insulating material) greatly amplifies the influence of the spin-orbit interaction on the surface properties. The best known manifestation of this effect is the momentum-dependent splitting of the surface state energies (Rashba effect). Here we show that the same interaction also generates a spin-polarization of the bulk states when an electric current is driven through the bulk of the film. For a jellium model of the bulk, which is representative of metals with a closed Fermi surface, we prove as a theorem that, regardless of the shape of the confinement potential, the induced surface spin density at each surface is given by $S = -\gamma\,(h/2\pi)\,\mathbf{z}\times\mathbf{j}$, where $\mathbf{j}$ is the particle current density in the bulk, $\mathbf{z}$ is the unit vector normal to the surface, and $\gamma = h/(8\pi mc^2)$ contains only fundamental constants. For a general metallic solid, the form of the surface spin density remains the same, while γ becomes a material-specific parameter that controls the strength of the interfacial spin-orbit coupling. Our theorem, combined with an ab initio calculation of the spin polarization of the current-carrying film, enables a determination of γ, which should be useful in modeling the spin-dependent scattering of quasiparticles at the interface.

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Taming Spins in a Band-gap Engineered Germanium by Light Touch

S.Hayashi[1], T.Tayagaki[2], Y.Okawa[1], Y.Yasutake[1,3], H.Yaguchi[4], Y Kanemitsu[2], and S.Fukatsu[1]

[1] Grad. School of A&S, University of Tokyo, Komaba, Meguro, Tokyo 153-8902, Japan
[2] ICR, Kyoto University, Uji, Kyoto 611-0011, Japan, [3]JST, Kawaguchi, Saitama 332-0012, Japan, [4]Saitama University, Shimo-Okubo, Sakura, Saitama 338-8570, Japan

Tel: +81-3-5454-6754 Fax: +81-3-5454-6998
E-mail: cfkatz@mail.ecc.u-tokyo.ac.jp

The spin degree of freedom of electron arguably adds to the charge counterpart in the chip technology. As such, the ability to control electron spin polarization (ESP) is crucial. Fortuitously, Ge a Si ally is rediscovered to be more spin-aware than thought. Indeed, finite ESP can be conveniently created in Ge with circular-polarized light, not by electrical spin injection. Recently, valley-selective spin control was demonstrated in the conduction band valleys of Ge by exploiting such optical means for ESP creation. A clear dominance switch of *antiparallel* to *parallel* spin orientation was observed in terms of ESP inversion between the zone-center and indirect L-valleys as excitation energy was varied. The former (latter) occurred when all valence subbands were (only heavy-hole subband was) involved in a band-gap engineered Ge. The zero-crossing energy of ESP showed a clear quantum-confinement shift, indicating that one can control the magnitude and sign of ESP by simply tuning the band-edge in relation to the excitation energy. The result is also intriguing in that intervalley scattering of electrons is central to the control of ESP, which can reach 100% in principle. Besides these, issues like L-to-Γ spin back-transfer, longer-than-expected relaxation times of spins in the L-valley, ways to establish spatial selectivity of electron spins, and efficient valley-specific ESP pumping will be discussed from the optoelectronics and information processing points of view.

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Molecular Transistors

Hyunwook Song[1,2,] Takhee Lee[3], and Mark A. Reed[1]

[1] Yale University, New Haven, CT, USA;
[2] Kyunghee University, Yongin, Korea;
[3] Seoul National University, Seoul, Korea

Tel: +1 203 432 4306 Fax: +1 203 432 6420
email: mark.reed@yale.edu

Electron devices containing molecules as the active region have been an active area of research over the last few years. In molecular-scale devices, a longstanding challenge has been to create a true three-terminal device; e.g., one that operates by modifying the internal energy structure of the molecule, analogous to conventional FETs. Here we report[1] the observation of such a solid-state molecular device, in which transport current is directly modulated by an external gate voltage. We have realized a molecular transistor made from the prototype molecular junction, benzene dithiol, and have used a combination of spectroscopies to determine the internal energetic structure of the molecular junction, and demonstrate coherent transport.[2,3] Resonance-enhanced coupling to the nearest molecular orbital is revealed by electron tunneling spectroscopy, demonstrating for the first time direct molecular orbital gating in a molecular electronic device.

We further demonstrate that energetic orbital positions can be modified by appropriate endgroup and sidegroup substitutions. Modifications of endgroups allows the realization of complimentary single molecule FET devices. Systematic sidegroup substitutions of varying electronegativity allows a systematic engineering of orbital positions, analogous to threshold voltage control. These results enable the ability to separately determine the roles of intrinsic versus contact conductivities.

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Conductance Fluctuations in Graphene Nanoribbons

B. Liu, R. Akis, and D. K. Ferry

School of Electrical, Computer, and Energy Engineering
Arizona State University, Tempe, AZ 85287-5706, USA

Tel: +1 480 965 2570
email: ferry@asu.edu

Over the past few years, the amazing properties of graphene have led to predictions for its use in a variety of areas, not the least of which is in semiconductor devices. But, the transport is an important aspect of any possible application. At low temperature, fluctuations are observed in the conductance through nanoribbons. These fluctuations arise from the presence of a random potential in the semiconductor, which arises from e.g. impurities present in the material structure. In this work, we examine the nature of these fluctuations in nanoribbons using an atomic basis quantum transport simulation. We find that fluctuations are generally very weak in graphene, and are not universal in nature. In energy sweeps, the amplitude of the fluctuation increases almost linearly with the amplitude of the random potential, with a saturation occurring at a peak to peak amplitude of ~2.8 eV, e.g., of the order of the bond energy in graphene. These results agree with experiments which generally show much weaker fluctuations in graphene than in normal semiconductors.

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Graphene Terahertz Electronics and Optoelectronics: Device Concepts and Physics of Device Operation

Victor Ryzhii and Taiichi Otsiji

Research Institute for Electrical Communication, Tohoku University
Sendai 980- 8577, Japan

Tel: +81-242-222-379;
email: v-ryzhii@riec.tohoku.ac.jp

The unique properties of graphene layers (GLs), particularly the gapless energy spectrum, relatively strong interband absorption, and pronounced plasmonic effects, provide opportunities to use different GL-based structures in novel active and passive terahertz and optoelectronic devices. The possibility to use for the inter-GL barriers such materials as hBN, WS_2, and similar materials, opens up new prospects to create the devices with enhanced functional abilities.

We overview the concepts of several terahertz and optoelectronic devices based on single-, double-, and multiple-GL structures:

(i) Optical modulators, including those involving the resonant excitation of plasma oscillations;

(ii) Terahertz and infrared lasers using the interband intra- and inter-GL transition;

(iii) Interband and intraband detectors of terahertz and infrared radiation;

(iv) Plasmonic resonant terahertz photomixers.

Some of such devices were proposed and realized by different research groups as well as by us and our collaborators. Using the developed models of these devices, we demonstrate the features of their operation and characteristics and the ultimate performance. We show that different terahertz and optoelectronic GL-based devices under consideration can markedly surpass and supplement the devices based on the heterostructures made of the standard semiconductors.

We are grateful to M.S.Shur, V.Mitin, M.Ryzhii, A.Satou, A.Dubinov, and V.Aleshkin for fruitful collaboration.
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Metal Non-metal Transition in Multi-walled Carbon Nanotubes

M. Kida[1], N. Aoki[1], T. Nakanishi[2], J. P. Bird[3], D. K. Ferry[4], and Y. Ochiai[1]

[1] Graduate School of Advanced Integration Science, Chiba University, Japan

[2] National Institutes of Advanced Industrial Science and Technology, Tsukuba, Japan

[3] Department of Electrical Engineering, SUNY Buffalo, USA

[4] Department of Electrical Engineering, ASU, Tempe, USA

Tel: +81-43-290-3428 Fax: +81-43-290-3427
email: ochiai@faculty.chiba-u.jp

In order to clarify the device application in multi-walled carbon nano-tubes (MWNTs), metal-nonmetal (MNM) transition and the low temperature magneto-resistance (MR) have been studied. discussed. In case of the ten or more layers, the transport shows a MNM transition in doped semiconductors as well as bulk semiconductors. Further more, in the low-temperature magneto-resistance (MR), Aharanov-Bohm (AB) flux cancellation behavior and Altshuler-Aronov-Spivak (AAS) & AB oscillations have been observed. Therefore, we have analyzed the MR results in order to explore the relation between flux cancellation and carrier transports including determination of its activation energy and the angular dependence of the applied magnetic field. These results must be very important to reveal a connection between the nature of transport in single-walled nano-tubes (SWNTs) and MWNTs. Also, such these transport properties defined in MWNT experiment must also provide important information for their device applications of MWNTs, including in nano-scaled field effect transistors using MWNT.

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Understanding Nanoscale Transport in Transparent Conductors based on Hybrid 1D/2D Networks

Suprem Das, Kerry Maize, Sajia Sadeque, Amr Mohammed, Ali Shakouri, Muhammad A. Alam, and David B. Janes

Purdue University
West Lafayette, IN 47907, USA

Tel: +1 765 494 9263 Fax: +1 765 494 0811
email: janes@purdue.edu

Networks of 1D materials (e.g. metal nanowires) or 1D/2D hybrids (e.g. nanowires plus single-layer graphene) are of interest as high-performance, flexible transparent conductors or as materials for transistors and sensors. Transport through such networks are typically considered in terms of percolation (1D) or co-percolation between two layers (1D and 2D)[1,2]. The percolating transport is presumed linear and spatially homogenous, although, in practice, the devices operate in nonlinear regime and conduction pathways in both types of networks are spatially inhomogeneous. A high-resolution method to probe current pathways and resistive bottlenecks over relatively large areas can provide insights into the conduction mechanisms and potential methods to improve the sheet resistance at a given transparency. In this study, we utilized high-resolution thermoreflectance imaging (TRI) with submicron spatial and 50 mK temperature resolution to map self-heating and hot-spot formation due to current flow within networks. TRI allows quantification of heterogeneity in transport including both qualitative and quantitative differences between networks of 1D materials and hybrid 1D/2D networks. Hot spots represent resistive bottlenecks, and super-Joule heating is observed at these junctions. The results encourage a fundamental reevaluation of the transport models and characterization results for network-based percolating conductors.

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Transmission Line Model for Microwave Fast Scanning Tool: Theoretical Backgrounds for Nanotube Nano-Characterization

Slava V. Rotkin[1], Eric Seabron[2], Scott Maclaren[2], Xu Xie[2], John A. Rogers[2], and William L. Wilson[2]

[1] Department of Physics, Lehigh University, Bethlehem, PA 18015, USA;
[2] Department of Materials Science and Engineering, Frederick Seitz Materials Research Laboratory, UIUC, Urbana, IL 61801, USA

Tel: +1 610 758 3930
email: rotkin@lehigh.edu

Various Microwave Scanning Probe Microscopy (uW-SPM) has recommended itself as a versatile non-destructive characterization tool, capable to map electronic materials' properties with nanometer resolution [1]. Still, the theory of the method is in its rudimentary stage, especially when applied to low-dimensional objects, where the classical description may be invalid. On the other hand recent success in fabrication of nanotube (NT) ultra-small devices [2], circuits and systems [3] demands for such a technique. Here we develop on the theory of uW characterization of NT materials.

One-dimensional (1D) electronic structure of the NT allows for several non-classical physical effects associated with lower screening of Coulomb interaction in 1D. These manifest itself, for example, in quantum capacitance, ballistic transport, plasmonic excitations, to name just a few. In the paper we elaborate on how this interesting physics can be accommodated within rather simple and thus analytical "transmission line" model, still covering fundamentals of uW-SPM. Recently we worked out the theory of NT antenna effects and applied it to the problem of near-field EM coupling of NTs to a bulk material [4]. Extension of the model into RF domain and for a nanoscale conductive SPM tip is discussed in detail.

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Graphene Applications in Thermal Management of Advanced Electronics

Alexander A. Balandin

Department of Electrical and Computer Engineering and Materials Science and Engineering Program, Bourns College of Engineering, University of California – Riverside, CA 92521, USA

Tel: +1 951 827 2351 Fax: +1 951 827 2425
email: balandin@ee.ucr.edu

Graphene reveals extremely high thermal conductivity of above ~2000 W/mK at room temperature [1]. The intrinsic thermal conductivity of graphene can exceed that of basal planes of graphite provided that the graphene flake is large enough. Few-layer graphene films preserve the heat conduction properties better than semiconductor or metal films. The unique thermal properties of graphene are explained by the specifics of the acoustic phonon transport in 2D crystals. Given such excellent heat conduction properties of graphene it is interesting to investigate possible applications of this material in thermal management. In this talk I describe our recent results of graphene use in thermal interface materials [2], heat spreaders for high-power GaN transistors [3], thermal phase change materials [4], hybrid graphene-copper interconnects [5], and graphene laminate used as coatings for electronic packaging [6].

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Toward the Large-Area and Tailored Growth of Graphene on Different Substrates

T. Schumann, J. Wofford, M.H. Oliveira, Jr., M. Ramsteiner, U. Jahn, St. Fölsch, B. Jenichen, A. Trampert, L. Geelhaar, J.M.J. Lopes, and H. Riechert

Paul-Drude-Institut für Festkörperelektronik,
Hausvogteiplatz 5−7,
10117 Berlin, Germany

email: riechert@pdi-berlin.de

Graphene is a two-dimensional material exhibiting unique electronic properties that give it huge potential for future nanoelectronics. The envisioned use of this material in different applications depends on the development of processes that will permit its controlled synthesis on a variety of substrates. Therefore, research efforts focusing on this aspect have recently been intensified. In this contribution, our recent results on the controlled growth of graphene (as nanoribbons or extended 2D layers) over different templates will be presented. Two different approaches for the synthesis of epitaxial graphene have been investigated at the Paul-Drude-Institut: surface graphitization of SiC surfaces and molecular beam epitaxy (MBE). In the first case, large-area growth of mono- and bi-layer graphene offering high structural and electronic quality could be achieved. Additionally, the formation of graphene nanoribbons on SiC stepped surfaces has also been investigated. Based on a careful control of the layer-by-layer growth of graphene on SiC(0001), the modulation of the nanoribbons width could be realized. This is important since this type of nanostructure can offer an electronic band gap (required for instance for transistor applications), which is strongly dependent on its dimensions. Figure 1 illustrates an atomic force microscopy (AFM) image of bilayer graphene nanoribbons formed on surface steps of a SiC (0001) surface. In this case, the average width of the nanoribbons is around 35 nm.

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The other method employed by us, MBE, is particularly promising for the well-controlled growth of graphene. It usually does not involve catalytic surface processes (as in chemical vapor deposition), and thus holds promise for graphene synthesis not only on metals but also on insulators and semiconductors. The exact deposition rates and sub-monolayer thickness precision, as well as the high degree of purity and interface control, are additional advantages offered by this technique. It will be shown that state of the art structural quality could be achieved for layers prepared on a metallic surface. Raman analyses of graphene films on Ni/MgO(111) substrates (see Figure 2) proves that the material exhibits high crystalline quality. For growth on non-metallic templates (e.g. Al_2O_3), nano-crystalline graphene films of different thicknesses (from a single to few atomic layers thick - see Figure 3), which homogeneously cover the entire surface of two-inch wafers, could be prepared in a controlled manner. Interestingly, despite the nano-crystalline nature, the MBE-grown graphene on insulators possesses a epitaxial relation to the underlying substrate. We will discuss these and other results in terms of non-conventional mechanisms of epitaxy, such as van der Waals epitaxy and growth from below.

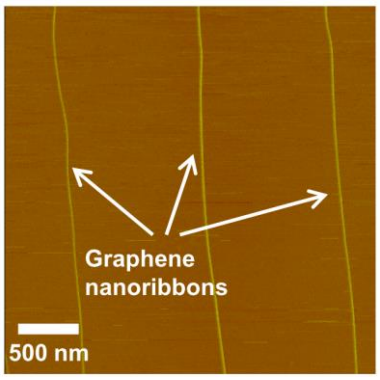

Fig. 1: AFM phase contrast image of bilayer graphene nanoribbons grown on SiC(0001) by the surface graphitization method. The average width of the nanoribbons in this case in ~ 35 nm.

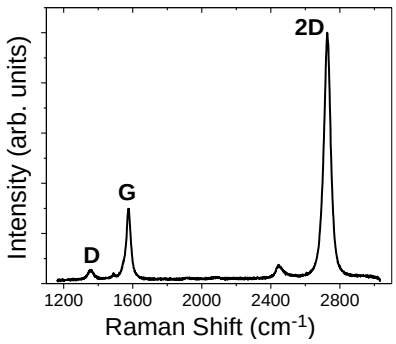

Fig. 2: Raman spectrum collected from graphene prepared on Ni/MgO(111) by MBE. The low intensity of the D peak is indicative of a very low defect concentration, and that individual domains are larger than 1μm.

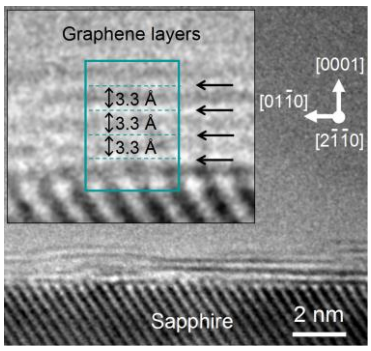

Fig. 3: Image obtained by transmission electron microscopy of a graphene film (few layers thick) prepared on Al_2O_3(0001) by MBE. The inset depicts a magnified image of the layers. The carbon layers are separated by 3.3 ± 0.2 Å, as expected for a stacking of few graphene layers.

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Direct Growth of Graphene on SiO_2 Substrate by Thermal & Laser CVDs

K. Matsumoto, T. Ikuta, K. Koshida, K. Maehashi, Y. Ohno, Y. Kanai, and K. Inoue

Osaka University,
8-1, Mihogaoaka, Ibaraki-shi,
Osaka-fu, 567-0047, Japan

Tel: +81-6-6879-8410, FAX: +81-6-6879-8410
email: k-matsumoto@sanken.osaka-u.ac.jp

We have succeeded in growing the graphene directly on the SiO_2/Si substrate using the amorphous carbon as a carbon source, where the thermal CVD and Laser CVD were applied. These technologies will be useful for the future device application of graphene.

On the SiO_2/Si substrate, 1nm amorphous carbon was deposited by the e-beam evaporation followed by the deposition of 30nm Ni metal as catalyst metal. For the thermal CVD, the Au or Pd metal are deposited on the Ni catalyst metal for the suppression of the segregation of Ni metal during the thermal process. In the H_2/Ar atmosphere of 2.6Pa, the sample was heated up to 700℃ to 870℃ for 10 minutes. After the cooling off, the catalyst metal was etched off and the graphene was formed directly on the SiO_2/Si substrate, which was confirmed by the Raman spectroscopy. The best condition of the heating process temperature is 850℃ and the highest mobility of 400m^2/Vs was obtained. For the Laser CVD, the substrate of Ni/amorphous carbon/SiO_2/Si substrate was preheated up to 200℃ for the assist of the growth. When the 9mW/μm^2 Ar laser of 514.5nm wavelength was irradiated to the substrate, the amorphous carbon was melted in to the catalyst metal of Ni. Because of the Laser power, the Ni metal was segregated and the melted carbon formed the graphene directly on the SiO_2/Si substrate. The formed graphene was confirmed by the Raman spectroscopy. This Laser CVD method can grow the graphene only anywhere device should be formed, and will be the useful tool for the future device applications.

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Scanning Tunneling Microscopy Studies of Graphene and Hydrogenated Graphene on Cu (111)

Shawna Hollen, Grady Gambrel, Steven Tjung, Ezekiel Johnston-Halperin, and Jay Gupta

Center for Emergent Materials, 191 W. Woodruff Ave.
The Ohio State University, Columbus, OH, USA
Tel: +1 614 688 0511, Fax: +1 614 292 7557,
email: hollen.8@osu.edu

The innate sensitivity of 2D material surfaces to their environment presents a challenge for applications that aim to employ the properties of the pristine materials, and at the same time an opportunity to design devices that exploit the surface sensitivity to tune electronic structure by functionalization. In particular, hydrogen functionalization of graphene to open a band gap is being widely researched because of its potential for lateral patterning of 2D devices. It is increasingly important to understand and characterize surface functionalization and interactions with environmental elements, such as substrate, metallic contacts, and adatoms. We developed a method for reproducible, epitaxial growth of pristine graphene islands on Cu(111) in UHV, and use scanning tunneling microscopy and spectroscopy (STM) to study the interaction of these graphene islands with the Cu substrate. Tunneling spectroscopy measurements of the electronic surface states over the graphene islands indicate a lower local work function, decreased coupling to bulk Cu states, and a decreased electron effective mass. Together, these results confirm expectations for graphene doping by metallic contacts, a relevant consideration for transport in devices. Additionally, we developed a novel field electron dissociation technique to form hydrogen-terminated graphene. This method produced what may be the first STM images of crystalline hydrogenated graphene. The pristine graphene island is then recovered by scanning at a high tip-sample bias. The hydrogenation and its reversibility suggest writing lateral 2D devices using the STM tip. Toward this end, we are developing the capability to repeat the hydrogenation on working graphene devices.

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A Molecular Design of Nonlinear Optical Properties and Conductivity Switches on the Basis of Open-shell Nature

Katsuki Okuno[1], Taku Takebayashi[1], and Yasuteru Shigeta[2,3]

[1] Graduate School of Materials Science, Osaka University, Toyonaka 560-8531, Japan

[2] Graduate School of Pure and Applied Science, University of Tsukuba, Tsukuba 305-8577, Japan

CREST Japan Science and Technology Agency, Kawagoe 332-0012, Japan.

Tel: +81-29-853-6496 Fax: +81-29-853-6496
email: shigeta@ccs.tsukuba.ac.jp

Open-shell singlet diradical molecules have been widely investigated because they are key to understanding the nature of chemical bonds. We propose a new concept for reversible switching of diradical character y, an index of the instability of chemical bonds, of a molecule by photochromic reaction. Photochromic diarylethene derivatives with various open-shell singlet diradical characters are theoretically designed, and their photochromic diradical character switching behaviors are clarified. These results contribute to designing highly efficient third-order nonlinear optical switching substances based on the correlation between the diradical character and second hyperpolarizability. We also investigated I-V characteristics of polyacenes, which are a kind of graphen nano-ribbons and exhibit open-shell nature when aromatic-ring units are long enough, as molecular conducting device and reveal the relationship between bias-dependent linear and nonlinear conductivities and the diradical character for a design of nanodevices.

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Transfer-Free Fabrication of Graphene Field Effect Transistor Arrays Using Patterned Growth of Graphene on a SiO_2/Si Substrate

Takashi Mizutani[1,2,3], Masato Tamaoki[1], Hideki Imaeda[1], and Shigeru Kishimoto[1]

[1] Department of Quantum Engineering, Nagoya University, Nagoya 464-8603, Japan
Furo-cho, Chikusa-ku,, Nagoya 464-8603, Japan

[2] Nagoya Industrial Science Research Institute,
1-3, Yotsuya-dori, Chikusa-ku, Nagoya 464-0819, Japan

[3] Institute for General Research of Science, Chubu University
1200, Matsumoto-cho, Kasugai 487-8501, Japan

Tel: +81-52-781-1883
email: takashimizutani@nagoya-u.jp

Transfer-free fabrication of graphene FET arrays has been successfully demonstrated using patterned growth of graphene on a SiO_2/Si substrate. The patterned growth of the graphene layer was achieved by depositing a tri-layered structure of a-C/Ni/Au in the channel area of the devices on a SiO_2/Si substrate[1], with subsequent graphitization annealing at 800 $^{\circ}$C for 15 min in a vacuum. The processes of graphene transfer onto an insulating substrate, and electrical isolation, have been eliminated by this patterned growth of the graphene. The source and drain electrodes were formed using conventional electron beam evaporation and lift-off technique. The heavily-doped Si substrate was used as a back gate. The device exhibited satisfactory current-voltage characteristics, with a mobility of 590 cm^2/Vs. Surface potential measurement of the graphene channel by Kelvin probe force microscopy showed little sign of electron-rich and hole-rich puddle formation[2], suggesting relatively uniform electrical properties. The present technology will open up a new possibility in implementing GFET integrated circuits with simple fabrication process.

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Non-Equilibrium First-Principles Study on Electron Scattering Processes in MTJ

Masaaki Araidai[1], Takahiro Yamamoto[2], and Kenji Shiraishi[1]

[1] Graduate School of Engineering, Nagoya University
Furo-cho, Chikusa-ku, Nagoya, 464-8603, Japan

[2] Faculty of Engineering, Tokyo University of Science
6-3-1 Niijuku, Katsushika-ku, Tokyo 125-8585, Japan

Tel: +81-52-789-4546 Fax: +81-52-789-4546
email: araidai@cse.nagoya-u.ac.jp

Current-induced magnetization switching (CIMS) [1,2] is a promising mechanism of magnetization switching in magnetoresistive random access memory. Although electron scattering processes through a MTJ are directly related to CIMS, it has not yet been studied well. Accordingly, we investigated CIMS in a MTJ by non-equilibrium first-principles calculations [3]. We employed an Fe/MgO(001)/Fe MTJ with a tantalum lead as the calculation model, as shown in the Fig. 1. A large TMR ratio was obtained even for the MTJ model with a thin magnetization switching layer. We found that the change in the magnetization configuration from antiparallel (AP) to parallel (P) can be realized with a lower electrical power than that from P to AP. From detailed analyses of the density of states subject to a finite bias voltage, we clarified that the asymmetric behavior originates from the difference in the electron scattering processes between switching directions.

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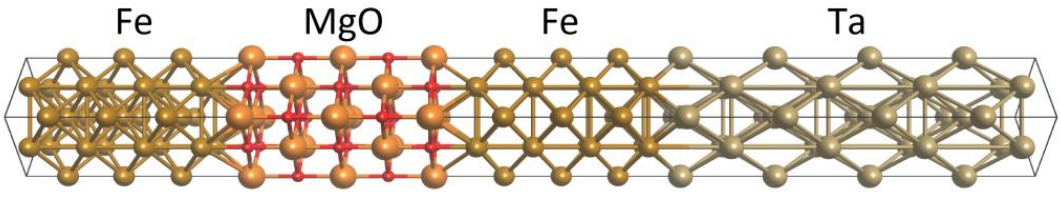

Fig.1 Calculation model of an Fe/MgO(001)/Fe MTJ with a paramagnetic Ta lead. Periodic boundary conditions are imposed in the directions parallel to the layers. The magnetization in the iron electrode attached to the leftmost Fe layer is fixed at the bulk value, and that in the thin iron layer is optimized according to the tunneling current through the junction.

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Forming of Electrons Wave Packets in Nano Scale Device

Genki Fujita[1], Taro Shiokawa[1], Yukihiro Takada[2], Satoru Konabe[1,7], Masakazu Muraguchi[4,5], Takahiro Yamamoto[3], Tetsuo Endoh[4,5], Yasuhiro Hatsugai[1,4], and Kenji Shiraishi[1,4,6]

1 Graduate School of Pure and Applied Sciences, University of Tsukuba, 1-1-1 Tennodai, Tsukuba, 305-8577, Japan
2 College of Science and Engineering, Aoyama Gakuin University, Shibuya, Tokyo, 150-0002, Japan
3 Faculty of Engineering, Tokyo University of Science, Chiyoda, Tokyo, 125-8585, Japan
4 Center for InnovaLve Integrated Electronic Systems, Tohoku University, Sendai, 980-8577, Japan
5 Graduate School of Engineering, Tohoku University, Sendai, 980-8579, Japan
6 Graduate School of Engineering, Nagoya University, Nagoya,464-8603, Japan
7 CREST, Japan Science and Technology Agency

Tel: +81 29 853 5600 8233
email: gfujita@comas.frsc.tsukuba.ac.jp

Recently, device size is miniaturized and the channel length will reach 10 nm in the most advanced research. It is inappropriate to treat electrons as particles in the very short channel length, while it is unreasonable to consider electrons as waves because of a high electric field expected in the next generation electron devices. In this work, we treat electrons as wave packets to describe a crossover feature between particle and wave nature. We investigate dynamics of electron wave packets under long-range Coulomb interactions and consider transport properties of many electrons that have both particle and wave characteristics by solving the time-dependent Hartree-Fock equation.

Our calculated results show that electrons tend to form electron wave packets at the boundary between source and channel region. Furthermore, behavior of electron transport in nano channels is sensitive to the strength of Coulomb interaction. These facts might be crucial for considering future nano-device properties.

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Hot-carrier Photodetector Beyond Spectral Limit

A. G. Unil Perera

Department of Physics and Astronomy,
Georgia State University, Atlanta, GA 30303, USA

Tel: +1 404 413 6037
email: uperera@gsu.edu

The hot-carrier dynamics is the subject of many studies in semiconductor physics and devices. Hot-carrier relaxation typically leads to energy dissipation into heat. Making use of the hot-carrier dynamics in a process contrary to conversion into heat should improve the energy efficiency. We have demonstrated an unusual extension of the spectral threshold wavelength into the very-long wavelength infrared (VLWIR) range in a GaAs/AlGaAs heterojunction photodetector, owing to energy transfer from hot carriers to cold carriers. An apparent advantage of this is setting apart the determination of spectral response and dark current by the same activation energy (Δ). A p-type GaAs/AGaAs heterojunction detector with Δ = 0.32 eV showing a response up to 100 μm has been demonstrated, whereas without the hot-carrier effect the threshold should correspond to ~3.9 μm. So far the highest operating temperature achieved is 35 K, which could be in part due to the fast relaxation process in bulk materials (sub-picoseconds). In place of the bulk materials using quantum structures (e.g., quantum well/dots/ring) should be lead to longer carrier lifetime.

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Optical Properties of Semipolar InGaN/GaN Quantum Wells Studied on the Nanoscale

Saulius Marcinkevicius[1], Kristina Gelzinyte[1], Ruslan Ivanov[1], Yuji Zhao[2], Shuji Nakamura[2], Steven P. DenBaars[2], and James S. Speck[2]

[1] Department of Materials and Nano Physics, KTH Royal Institute of Technology
Electrum 229, 16440 Kista, Sweden

[2] Materials Department, University of California
Santa Barbara, CA 93106, USA

Tel: +46 8 7904192 Fax: +46 8 7896672
email: sm@kth.se

Semipolar InGaN/GaN quantum wells (QWs) have a great potential to become the basis of energy efficient LEDs and lasers, especially in the green spectral region. Compared to conventional polar structures, they have smaller intrinsic electric fields and a good In uptake, allowing to reach longer wavelengths. Still, to assess the intrinsic limitations of semipolar InGaN QWs, several issues, such as the role of localized states and features of carrier recombination remain to be understood.

In the present work, scanning near-field optical microscopy (SNOM) and time-resolved photoluminescence techniques were applied to examine light polarization, rates of radiative and nonradiative recombination, and spatial distribution of band gap variations in single $(20\bar{2}1)$ and $(20\bar{2}\bar{1})$ QWs of different alloy compositions.

SNOM scans revealed that spatial band gap variations are small (tens of meV), and islands of uniform potentials are large (a few μm). Recombination properties were spatially uniform, and carrier redistribution between different potential sites weak, which suggests that semipolar InGaN QWs are prone to hot spot formation in light emitting devices. Radiative recombination prevailed up to ~200 K. At higher temperatures, nonradiative recombination was more efficient. Still, room temperature carrier lifetimes were in the ns range, which is important for light emitting applications.

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Reliability Modelling of CdTe Photovoltaics

Dragica Vasileska[1], Da Guo[1], Igor Sankin[2], Tian Fang[2], Richard Akis[1], Christian Ringhofer[1], and Daniel Brinkman[1]

[1]Arizona State University
Tempe, AZ 85287-5706, USA

[2]First Solar, Perrysburg, OH 43551, USA

e-mail: vasileska@asu.edu

Thin-film modules of all technologies often suffer from performance degradation over time. Some of the performance changes are reversible and some are not, which makes deployment, testing, and energy-yield prediction more challenging. Manufacturers devote significant empirical efforts to study these phenomena and to improve semiconductor device stability. Still, understanding the underlying reasons of instabilities remains clouded due to the lack of ability to characterize materials at the atomistic levels and lack of the interpretation from the most fundamental material science. The most commonly alleged causes of metastability in CdTe device, such as "migration of Cu," have been interrogated rigorously over the past fifteen years. Still, the discussions often ended prematurely by stating observed correlations between stress conditions and changes in atomic profiles of impurities or CV doping concentrate-on. *Multiple hypotheses suggesting degradation of CdTe solar cell devices due to interaction and evolution of point defects and complexes were proposed, and none of them received strong theoretical or experimental confirmation.*

The novelty of the work that will be presented at the workshop is that the Unified 1D Solver, developed as part of the DOE PREDICTS project, enables improved prediction of long-term solar-cell performance as well as the separation of reversible and irreversible changes. Overall, the confidence in the prediction of thin-film module reliability with this tool has the opportunity to move away from empirical observation to scientific understanding. Based on the detailed understanding, approaches are proposed to overcome the long-term instability of the CdTe solar cell under stress.

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Ultrafast Carrier Relaxation in Nanowire Structures for Photovoltaic Applications

Raghuraj Hathwar, Yongjie Zou, Christiana Honsberg, Paolo Lugli, Marco Saraniti, and Stephen Goodnick

School of Electrical Computer and Energy Engineering
Arizona State University
Tempe, AZ 87287, USA
e-mail: stephen.goodnick@asu.edu

Advanced concept solar cells are of current interest in improving the efficiency of current photovoltaic technology beyond the single bandgap Shockley-Queisser efficiency limit. Several advanced concept approaches are currently under investigation by a variety of groups, including quantum well, nanowire and quantum dot systems for multi-exciton generation (MEG) and hot carrier solar cells. Here we investigate the short time carrier dynamics in semiconductor nanowires under varying photoexcitation conditions using full band Cellular Monte Carlo (CMC) simulation coupled with thermodynamic models, to understand the limiting factors affecting solar cell performance. The CMC code is used to simulate the dynamics of photoexcited electrons in the quantum confined states III-V nanowire systems using an atomistic tight binding representation of the nanowires. Scattering processes due to optical phonons (polar and nonpolar) and acoustic phonons are included. In particular, we look at the energy relaxation rate in connection with MEG in semiconductor nanowire systems, and the feasibility of nanowire solar cells incorporating MEG. The carrier relaxation dynamics were studied in strongly confined InAs NWs ($2\times2nm^2$ and $3\times3nm^2$) with carriers injected at $2E_g$ and $3E_g$, to look at the competition between thermal relaxation and impact ionization at the critical energies for MEG to occur. Due to the large number of quasi-1D subbands at high excitation energy, the initial relaxation in InAs NWs is relatively fast, similar to bulk InAs, whereas the relaxation rate is reduced as carrier reach the ground subband, evidencing a phonon bottleneck effect. Future work will investigate the band to band impact ionization rate in III-V nanowires, for simulation of the quantum efficiency of the MEG process in realistic nanowire structures.

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Spin Pumping to Spin Seebeck Effects

E. Saitoh[1-3]

[1]WPI-AIMR, Tohoku University, Sendai 980-8577, Japan
[2]Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan
[3]ASRC, Japan Atomic Energy Agency, Tokai 319-1195, Japan

Tel: +81-(0)22-215-2021 Fax: +81-(0)22-215-2020
email: eizi@imr.tohoku.ac.jp

Spin current, a flow of electrons' spins in a solid, is the key concept in spintronics that will allow the achievement of efficient magnetic memories, computing devices, and energy converters. I here review phenomena which allow us to use spin currents in insulators [1]: inverse spin-Hall effect [2,4], spin pumping, spin-Hall magnetoresistance (SMR) [7], and spin Seebeck effect [4-6]. We found that spin pumping and spin torque effects appear at an interface between an insulator YIG and Pt. Using this effect, we can connect a spin current carried by conduction electrons and a spin-wave spin current flowing in insulators. We demonstrate electric signal transmission by using these effects and interconversion of the spin currents [1]. Seebeck effect (SSE) is the thermal spin pumping [5]. The SSE allows us to generate spin voltage, potential for driving nonequilibrium spin currents, by placing a ferromagnet in a temperature gradient. Using the inverse spin-Hall effect in Pt films, we measured the spin voltage ge nerated from a temperature gradient in various ferromagnetic insulators.

This research is collaboration with K. Ando, K. Uchida, Y. Kajiwara, S. Maekawa, G. E. W. Bauer, S. Takahashi, and J. Ieda.

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Experimental Demonstration of Magnonic Holographic Memory

Frederick Gertz[1], Alexander Kozhevnikov[2], Yuri Filimonov[2], and Alexander Khitun[1]

[1] Electrical Engineering Department, University of California - Riverside, Riverside, CA 92521, USA
[2] Kotel'nikov Institute of Radioengineering and Electronics of Russian Academy of Sciences, Saratov Branch, Saratov 410019, Russia

Tel: +1 951 827.5816 Fax: +1 951 827.2425
email: akhitun@engr.ucr.edu

Collective oscillation of spins in magnetic lattice known as spin waves (magnons) possess relatively long coherence length at room temperature, which makes it possible to build sub-micrometer scale holographic devices similar to the devices developed in optics. In this work, we present experimental data on a prototype 2-bit magnonic holographic memory. The prototype consists of the double-cross waveguide structure made of $Y_3Fe_2(FeO_4)_3$ with cobalt magnets placed on the top of waveguide junctions. It appears possible to recognize the state of each magnet via the interference pattern produced by the spin waves. The potential advantage of the spin wave approach is that the operating wavelength can be scaled down to the nanometer scale, which translates in the possibility of increasing data storage density to 1Tb/cm^2. The development of magnonic holographic memory devices and their incorporation within integrated circuits may pave a road to the next generation of logic devices exploiting phase in addition to amplitude for logic functionality.

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Self-Polarized Spin-Nanolasers

Ju-Ying Chen, Tong-Ming Wong, Che-Wei Chang, Chen-Yuan Dong, and Yang-Fang Chen

National Taiwan University
No. 1, Sec. 4, Roosevelt Road, Taipei, 10617 Taiwan (R.O.C)

Tel: +886-2-3366-5125 Fax: +886-2-2363-9984
email: yfchen@phys.ntu.edu.tw

The manipulation of spin in spin-lasers adds an new dimension to develop novel multifunctionality with better performance than their conventional counterparts. However, the rigid requirements of weak spin relaxation and efficient spin injection remain great challenges. Here, we show that these difficulties can be circumvented by using a new self-polarized spin mechanism. We demonstrate that a high degree of circular polarization of self-polarized spin-nanolasers up to 28.2 % can be achieved at room temperature in a low magnetic field of 0.35 T based on periodic GaN nanorods arrays and Fe_3O_4 nanoparticles. The unique energy band alignment of Fe_3O_4 nanoparticles for spin up and spin down electrons spontaneously generates the population imbalance of spin down and spin up electrons in GaN nanorods without an external bias due to selective spin charge transfer. Therefore, electrical pumping by magnetic electrode or optical pumping by circularly polarized light are not required. The methodology shown here can open up a new route to a variety of material systems for the effective generation of spin-lasers covering a wide range of spectrum.

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Pushing a Non-Volatile Magnetic Device Structure Towards a Universal CMOS Logic Replacement

Thomas Windbacher, Alexander Makarov, Viktor Sverdlov, and Siegfried Selberherr

Institute for Microelectronics, TU Wien
Gußhausstraße 27-29, A-1040 Wien, Austria

Tel: +43-1-58801-36010, Fax: +43-1-58801-36099
email: Selberherr@TUWien.ac.at

The soaring investment costs and the ever increasing severeness of physical limits for upcoming CMOS technology nodes will bring CMOS shrinking to a halt in the foreseeable future. Spintronics is a promising way to circumvent these obstacles, due to its non-volatility, high endurance, and fast operation. Promising results with respect to speed and power consumption have been already shown [1-3]. However, the introduced magnetic tunnel junctions (MTJs) act as mere auxiliary devices and require additional circuits for their operation, while the actual computation is carried out via CMOS transistors.

Our non-volatile magnetic flip-flop is capable of performing logic operations within the magnetic domain, which leads to a very small circuit foot print [4]. An extremely dense layout is achieved, when the device is extended to a non-volatile magnetic shift register [5]. Additionally the device structure intrinsically features a bias field free spin torque nano-scale oscillator [6] and can be combined with spin torque majority gates [7] to further boost the integration density. Thus, the proposed structure constitutes a very versatile and viable building block for a universal post CMOS logic technology.

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New Design of Spin-Torque Nano-Oscillators

Alexander Makarov, Thomas Windbacher, Viktor Sverdlov, and Siegfried Selberherr

Institute for Microelectronics, TU Wien
Gußhausstraße 27-29, A-1040 Wien, Austria

Tel: +43-1-58801-36033 Fax: +43-1-58801-36099
email: Sverdlov@iue.tuwien.ac.at

New types of spintronic devices based on MgO magnetic tunnel junctions (MTJs) with a large magneto-resistance ratio and utilizing all-electrical magnetization manipulation by current, such as spin-torque transfer RAM and spin-torque oscillators, have been successfully developed [1]. Spin-torque oscillators built on MTJs with an in-plane magnetization show high frequency capabilities, but still need an external magnetic field and are characterized by a low output power level [2]. Oscillators on MTJs with a perpendicular magnetization and vortex-based oscillators are able to generate oscillations without an external magnetic field, however, their low operating frequencies, usually below 2GHz, limit their functionality and application as tunable oscillators [2]. In [3] we proposed a bias field-free spin-torque oscillator based on an in-plane MgO-MTJ with a free magnetic layer of an elliptical cross-section not perfectly overlapping with a fixed magnetic layer of a smaller cross-section. However, a disadvantage of such a structure is a very narrow range of frequencies and their weak dependence on the current density. In [4] we presented a novel design of spin-torque oscillators composed of two penta-layer in-plane MgO-MTJs with a common free layer shared by both MTJs. This structure operates without a biasing field at high frequencies. Here we investigate in detail a variation of such a structure: a spin-torque nano-oscillator composed of two three-layer in-plane MgO-MTJs with a shared free layer, in particular the optimization in order to obtain maximum output power.

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