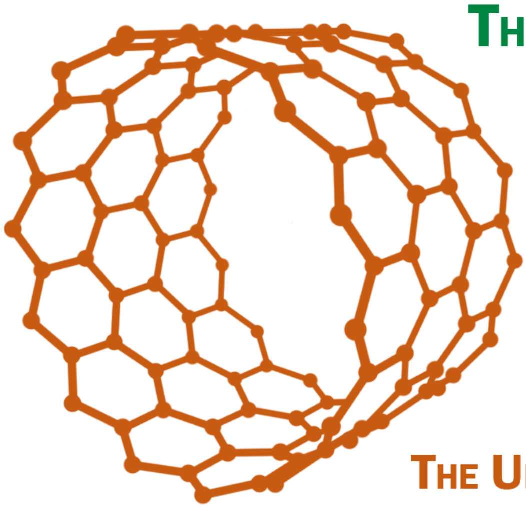
University of Texas at Dallas
Materials Science and Engineering
School of Engineering and Computer Science

72nd Physical Electronics Conference

On
The Physics and Chemistry of Surfaces and Interfaces



THE 72ND
Physical
Electronics
Conference
June 2012
THE UNIVERSITY OF TEXAS AT DALLAS

June 3 – 6, 2012
Richardson, Texas

Program
Abstracts
Conference Information

72nd Annual Physical Electronics Conference
Final Program

A Topical Conference on the Physics and Chemistry of Surfaces and Interfaces
72nd Annual Meeting, June 3 – 6
Department of Materials Science and Engineering
University of Texas at Dallas, Richardson, Texas

Sponsored by:

- American Elements
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The PEC organizers enthusiastically acknowledge and thank the following organizations for their support:

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About PEC

The Physical Electronics Conference has been held on university campuses and at research labs around North America for more than 70 years. This topical conference provides an annual forum for the dissemination and discussion of new research results in the physics and chemistry of surfaces and interfaces. The conference emphasizes fundamental science in materials systems, including metals, semiconductors, insulators and biomaterials.

Each year physicists and chemists with interests in these fields come together to solicit papers on experimental and theoretical research performed at exposed (gas-solid), buried (liquid-solid and solid-solid) and hybrid (e.g., semiconductor-biomaterial) interfaces. Representative topics include electronic, chemical, magnetic and structural properties of interfaces; kinetics and dynamics of physical and chemical transformations at surfaces; formation, modeling and properties of nanoscale-mesoscale surface architectures; correlated electron effects at surfaces; biological interactions with surfaces; mechanisms of surface and interface growth and evolution; and energy and electron transfer processes across materials interfaces. Properties of structurally and chemically tailored surfaces are of interest, as are new methods of measuring these properties and the demonstration of new applications.

Previous Physical Electronic Conference Hosts

1966	Massachusetts of Technology
1967	Massachusetts of Technology
1968	University of Minnesota
1969	Yale University
1970	University of Wisconsin-Milwaukee
1971	National Bureau of Standards
1972	Sandia Laboratories
1973	University of California at Berkeley
1974	Bell Laboratories
1975	Pennsylvania State University
1976	University of Wisconsin - Madison
1977	Stanford University
1978	Oak Ridge National Laboratory
1979	University of Maryland
1980	Cornell University
1981	Montana State University
1982	Georgia Institute of Technology
1983	Sandia Laboratories
1984	Princeton University
1985	University of Wisconsin-Milwaukee
1986	University of Texas at Austin
1987	IBM Almaden Research
1988	Brookhaven National Laboratory
1989	University of Washington
1990	National Bureau of Standards
1991	Rutgers University
1992	University of California at Irvine
1993	Rensselaer Polytechnic Institute
1994	University of Tennessee
1995	Arizona State University
1996	Boston University
1997	University of Oregon
1998	Pennsylvania State University
1999	University of California at Berkeley
2000	Louisiana State University
2001	Sandia National Laboratories
2002	Georgia Technical
2003	Cornell University
2004	University of California at Davis
2005	University of Wisconsin - Madison
2006	Princeton University
2007	University of Illinois at Champaign- Urbana
2008	University of California at Riverside
2009	Rutgers University
2010	University of Wisconsin-Milwaukee
2011	University of Albany

Nottingham Prize

The Nottingham Prize was originally established in 1966 from contributions given in memory of Professor Wayne B. Nottingham of the Massachusetts Institute of Technology, by his many friends and associates. The prize, currently consisting of a certificate and $1,000, is awarded to the best student paper, based on a PhD thesis, presented at the conference. This prize represents a seminal honor since many Nottingham winners have gone on to become leaders in the field of surface science.

Previous Nottingham Prize Winners

Year	Winner	Institution	PI
1966	L. F. Cordes	University of Minnesota	W. T. Peria
1967	D. Steiner	Massachusetts Institute of Technology	E. P. Gyftopoulos
	J.V. Hollweg	Massachusetts Institute of Technology	E. P. Gyftopoulos
1968	E. Ward Plummer	Cornell University	T. N. Rhodin
1969	John C. Tracy	Cornell University	J. M. Blakely
1970	J. M. Baker	Cornell University	J. M. Blakely
1971	D. P. Smith	University of Minnesota	W. T. Peria
1972	W. Henry Weinberg	University of California, Berkeley	R. Merrill
1973	J. R. Bower	Bartol Research Foundation	J. M. Chen
1974	N. J. Dionne	Cornell University	T. N. Rhodin
	Torgny Gustafsson	Chalmers University of Technology	P. O. Nillson
1975	L. C. Isett	Cornell University	J. M. Blakely
1976	J. A. Knapp	Montana State University	G. A. Lapeyre
1977	S.-L. Weng	University of Pennsylvania	E. W. Plummer
1978	Gwo-Ching Wang	University of Wisconsin, Madison	M. G. Lagally
1979	Wilson Ho	University of Pennsylvania	E. W. Plummer
1980	R. DiFoggio	University of Chicago	R. Gomer
	Harry J. Levinson	University of Pennsylvania	E. W. Plummer
1981	Ruud M. Tromp	FOM Institute for Atomic & Molecular Physics	F. W. Saris
1982	P. O. Hahn	University of Hanover	M. Henzler
1983	R. Raue	Cologne and KFA Julich	G. Guntherodt & M. Campagna
1984	M. Onellion	Rice University	G. K. Walters
1985	K. Gibson	University of Chicago	S. J. Sibener
	J. W. M. Frenken	FOM Institute for Atomic & Molecular Physics	J. F. van der Veen

1986	S. M. Yalisove	University of Pennsylvania	W. R. Graham
1987	John D. Beckerle	Massachusetts Institute of Technology	S. T. Ceyer
1988	Lee J. Richter	Cornell University	W. Ho
1989	J.-K. Zuo	Rensselaer Polytechnic Institute	C.-C. Wang
1990	Y.-W. Mo	University of Wisconsin, Madison	M. G. Lagally
1991	Brian S. Swartzentruber	University of Wisconsin, Madison	M. B. Webb
1992	Thomas Michely	KFA, Julich	G. Comsa
1993	A. K. Swan	Boston University	M. El-Batanouny
1994	G. Rosenfeld	KFA, Julich	G. Comsa
1995	Marcus K. Weldon	Harvard University	C. Friend
1996	J. Carpinelli	University of Tennessee	E. W. Plummer
	B. Kohler	Fritz Haber Institute	M. Scheffler
1997	D. Gragson	University of Oregon	G. Richmond
1998	Barry C. Stipe	Cornell University	W. Ho
	M. S. Hoogeman	FOM Institute & Leiden Univ.	J. W. M. Frenken
1999	K. Pelhos	Rutgers University	T. E. Madey
2000	Lincoln Lauhon	Cornell University	W. Ho
2001	Gayle Thayer	University of California, Davis & Sandia Livermore	S. Chiang & R. Hwang
2002	Denis Potapenko	Rutgers University	B. J. Hinch
2003	John Pierce	University of Tennessee	E. W. Plummer & J. Shen
2004	Peter Wahl	Max Planck Institute for Solid-State Physics	Klaus Kern
2005	Nathan Guisinger	Northwestern University	Mark Hersam
2006	Mustafa Murat Ozer	University of Tennessee-Knoxville	J. R. Thompson & H. H. Weitering
	Paul C. Snijders	Delft University of Technology	H.H. Weitering & T.M. Klapwijk
2007	Peter Maksymovych	University of Pittsburgh	J. T. Yates, Jr.
2008	Brett Goldsmith	University of California, Irvine	P. G. Collins
2009	Alpha T. N' Diaye	University of Köln (Cologne)	Thomas Michely
2010	Heather Tierney	Tufts University	Charlie Sykes
2011	Tanza Lewis	University of California, Irvine	John Hemminger & Bernd Winter

Emergency Contact Phone Numbers (for Sunday):

Dr. Chabal:	732-406-0335
Dr.Jean-Francois (Jeff) Veyan	214-484-5283 or 469-888-3542
Dr. Oliver Seitz	732-841-7947
Housing:	972-883-5241

Addresses:

Campus housing: University Village Residence Hall North
2851 Rutford Ave.
Richardson, TX 75080

NSERL Building: 813 Synergy Park Blvd.
Richardson, TX, 75080

Connecting to the campus internet:

The following is an instruction set for connecting to *UTDGuest,* an unencrypted wireless network here at UT Dallas. (https://wiki.utdallas.edu/wiki/display/IRDOCS/UTD+Guest+Unencrypted+Network)

Connecting to UTDGuest:

Step #1) Double click **Wireless Network Connection** into your system tray.

Step #2) Select *UTDGuest* from the available wireless networks and click **Connect**

Step #3) A message will appear explaining that you're connecting to an unencrypted network. The *UTDGuest* wireless network is not encrypted, so click **Connect Anyway**.

Step #4) The connection process should be quick. Once connected, you should see *Connected* beside the *UTDGuest* wireless network in **Wireless Network Connections**.

Step #5) You are connected at this point and may browse the internet. When you open your internet browser, you will have to click *Accept*, after reading the page top to bottom.

Step #6) You are now free to roam the internet.

Local Transportation

Taxi

Taxis are readily available at both airport locations. A few local taxi companies are listed below:

- Yellow Cab: 214-426-6262
- Alamo Cab: 214-688-1999
- Checker Cab: 972-222-2000

Ride the Comet Cruiser (DART Route 883)

Description of Service

The University operates campus shuttle bus services to provide on- and off-campus transportation to students, faculty, staff, and visitors that are convenient, cost effective, and safe. Services are operated in cooperation with Dallas Area Rapid Transit (DART) and serve the local community.
Route 883 provides transit service Monday through Saturday connecting the University to the DART Light Rail system and local residential and shopping areas. Route and schedule information can be found below.

All transit services operated by the University are free to all riders and open to the public.

No pass or identification of any sort is necessary. You can use the online DART Trip Planner to create personalized trip plans, customized schedules, and to find the DART stops nearest to your location.

How to Ride

First check for route maps and schedules.
Next go to the nearest bus stop to your origination. Make sure you are at an official DART bus stop displaying the proper route number. Note that times given on the bus schedule are the times at which the bus will leave the stop, make sure you arrive at the bus stop a few minutes before the next scheduled leave time. Buses run on official U.S. Government time. The bus will only pick you up if you are waiting at a designated DART bus stop. When the bus arrives please enter the bus through the front door only. Allow other passengers to get off before boarding. Sit anywhere you like. Generally, seats near the front door are reserved for elderly and mobility-impaired passengers. You may carry on baby strollers, carts, and other small items; just make sure they don't block the aisle.

If you need to access the bus by wheelchair, each bus is equipped with an automatic lift located at the front door. Please ask the driver for assistance with the lift. Guide dogs and other service animals are permitted on the bus. Buses are also equipped with bicycle racks.

Be seated, relax, and watch for your destination. If you are standing, stand behind the yellow line at the front of the bus and never stand or sit in the stairwells of the bus. En route, buses stop only at designated stops and only when a rider needs to board or get off the bus. Signal the driver that you want to get off at the next stop by pulling the cord installed just above the windows. Please pay attention so that you do not miss your stop because once the bus has pulled away from the stop the driver cannot stop again to let you off.

Exit through the front or rear doors. The operator will open the front door. Let the driver know if you need to exit through the rear door. When you exit the bus check around for any belongings you brought with you. The University is not responsible for items left on the bus. After exiting the bus, walk behind the bus and always use a crosswalk to cross the street.

Week days buses leave every 20 minutes:

Westbound (Rutford Southbound)	Bush Turnpike Station -	7:00 AM	Last Bus 10:40 PM
	UTD Berkner	7:20 AM	Last Bus 11:00 PM
	McCallum Bvd.	7:40 AM	Last Bus 11:00 PM
Eastbound (Rutford Northbound)	McCallum Blvd.	7:00 AM	Last Bus 10:40 PM
	UTD Berkner	7:20 AM	Last Bus 11:00 PM
	Bush Turnpike Station	7:40 AM	Last Bus 11:00 PM

Schedules are subject to change without notice. Traffic conditions or bad weather may adversely affect running times. Please check this website regularly for updates and information on holidays or special events.

Contact (972) 883-7777 or visit the Comet Cruiser website for more information on UT Dallas 883 Comet Cruiser bus service. Follow on Twitter, or send "follow @utdcometcruiser" to 40404 to get updates via text message when there is a new Twitter update. Standard text message rates apply.

2012 Physical Electronics Conference Program

All oral presentations are in the Davidson Auditorium (JSOM 1.118) located in the Naveen Jindal School of Management (JSOM) building. Breaks, vendors, and registration will be in the JSOM Atrium, just outside the auditorium. Posters and vendors will be displayed in the Galaxy Rooms, located in the Student Union (SU 2.602). Lunch will be served in the Galaxy Rooms

Sunday, June 3, 2012

3:00 – 5:00 PM	Dorm check-in – Residence Hall North - lobby (to check-in to your dorm room after 5 p.m., please call 972-883-5241)
5:00 – 9:00 PM	Registration and Welcome Reception – NSERL(RL) lobby

Monday, June 4, 2012

7:30 – 8:30 AM	Registration and breakfast - JSOM Atrium
8:30 – 8:40 AM	Opening and Welcome – Davidson Auditorium
Session 1	**Oral Presentations – Davidson Auditorium**
Moderator:	*Lauren Webb, University of Texas at Austin*
8:40 – 9:00 AM	O-01. **Orientational Transition and Competitive Pathways in the Adsorption of Phenols on the Ge(100)-2 × 1 Surface** Bonggeun Shong[1] and Stacey F. Bent[1], [1] Department of Chemical Engineering, Stanford University
9:00 – 9:20 AM	O-02. **The Picture Tells The Story: STM Reveals The Mechanism of Silicon Oxidation** Melissa A. Hines[1], Marc F. Faggin[1], Kun Bao [1],Ankush Gupta[1], and Brandon A. Aldinger[1] [1] Department of Chemistry, Cornell University, Baker Laboratory
9:20 – 9:40 AM	O-03. **Activation of surface hydroxyl groups by modification of H-terminated Si(111) surfaces** Peter Thissen[1], Tatiana Peixoto[1], Roberto C. Longo[1], Wolf Gero Schmidt[2], Kyeongjae Cho[1] and Yves J. Chabal[1] [1] Department of Materials Science and Engineering, University of Texas at Dallas [2] Lehrstuhl für Theoretische Physik, Universität Paderborn, Germany

9:40 – 10:00 AM O-04. **Reaction Pathways Involved Chemical Bath Deposition of Lead Sulfide on Functionalized Self-Assembled Monolayers**
Jing Yang[1], Amy V. Walker[1]
[1]Department of Material Science and Engineering, University of Texas at Dallas

10:00 – 10:20 AM **Coffee Break** – JSOM Atrium

Session 2 Oral Presentations – Davidson Auditorium

Moderator: *Manuel Quevedo-Lopez, University of Texas at Dallas*

10:20 – 10:40 AM O-05. **High Quality Organic/Semiconductor Interface demonstrated by adding Al_2O_3 over the Organic Layer**
W. Peng[1], O. Seitz[1], R. A. Chapman, E. M. Vogel[2] and Y. J. Chabal[1]
[1]Material Science and Engineering, University of Texas at Dallas, [2]Material Science and Engineering, Georgia Institute of Technology,

10:40 – 11:00 AM O-06. **Effect of Oxygen on the Stability of Ag islands on Si(111)-(7x7)**
Dahai Shao[1,2], Xiaojie Liu[1,3], Ning Lu[1,3], C.-Z. Wang[1,3], Kai-Ming Ho[1,3], M.C. Tringides[1,3] and P.A. Thiel[1,2,4]
[1]Ames Laboratory[2]Department of Chemistry, Iowa State University
[3]Department of Physics and Astronomy, Iowa State University[4] Department of Materials Science and Engineering, Iowa State University,

11:00 – 11:20 AM O-07. **Structure Evolution in Microaerosol-Deposited PCBM Monolayer Films on Au(111)**
Q. Shao[1], L. Tskipuri[1] and J. Reutt-Robey[2]
[1] Department of Chemistry & Biochemistry, University of Maryland,

11:20 – 11:40 AM O-08. **Sub-monolayer Spin Rotation of Photoelectrons from FePC on Fe(110)**
J. E. (Jack) Rowe[1], Daniel B. Dougherty[1], Andreas Sandin[1] and Elio Vescovo[2]
[1] Department of Physics, North Carolina State University
[2] National Synchrotron Light Source, Brookhaven National Labs,

11:40 – 12:00 PM O-09. **Hydrogen-Related Defects in Strontium Titanate**
M. C. Tarun[1] and M. D. McCluskey[1]
[1] Department of Physics and Astronomy and Materials Science and Engineering Program, Washington State University

12:00 – 1:30 PM **Lunch Break – Galaxy Rooms (Student Union)**

Session 3 Invited and Oral Presentations – Davidson Auditorium

Moderator: *Luigi Colombo, Texas Instruments*

1:30 – 2:10 PM

INVITED: **Electronic Structure and Excitations at Organic Semiconductor Interfaces**
Oliver L.A. Monti[1]
[1]Department of Chemistry and Biochemistry, University of Arizona

2:10 – 2:30 PM

O-10. **Transition Metal Arenes for Graphene Molecular Doping**
A. Laracuente[1], D. Barlow[1], R. Stine[1], J. Robinson[1], V. Bermudez[1], T. Reinecke[1] and P. Sheehan[1]
[1]Naval Research Laboratory

2:30 – 2:50 PM

O-11. **Tunable Interface Electronic Properties at Metal-Graphene-Metal Sandwich Contacts**
C. Gong[1] R. Wallace, K. Cho[1], and Y. J. Chabal[1]
[1]Department of Materials Science and Engineering, University of Texas at Dallas

2:50 – 3:10 PM

O-12. **Low- κ organic layer as a top gate dielectric for graphene field effect transistors**
G. Mordi[1], S. Jandhyala[2] and J. Kim[2]
[1]Department of Electrical Engineering, [2]Department of Materials Science and Engineering, University of Texas at Dallas

3:10 – 3:30 PM

O-13. **Potential Steps at Nanophase-Separated C_{60}-TiOPc-Ag(111) Interfaces**
J. E. Reutt-Robey[1], K. M. Burson,[2] Y. Wei[1#], W. G. Cullen[2], and M. S. Fuhrer[2]
[1]Department of Chemistry & Biochemistry, University of Maryland
[2]Department of Physic, University of Maryland
[#]Current Address: iNANO and Dept. of Physics & Astronomy, Aarhus University, Denmark

3:30 – 3:50 PM

Afternoon Break – JSOM Atrium

Session 4 Oral Presentations – Davidson Auditorium

Moderator: *Christopher Hinkle, University of Texas at Dallas*

3:50 – 4:10 PM

O-14. **Oxygen-induced (3×1) reconstruction on InAs(100) surface: Stable In-O-In subsurface trilayer**
M.P.J. Punkkinen[1], P. Laukkanen[1], J. Lång[1], J. Dahl[1], L. Vitos[2] and K. Kokko[1]
[1]Department of Physics and Astronomy, University of Turku, Finland
[2]Applied Materials Physics, Department of Materials Science and Engineering, Royal Institute of Technology, Stockholm, Sweden

4:10 – 4:30 PM O-15. **Observation of Polar InN with Surface Fermi Level near Valence Band Maximum**
J. Dahl[1], M. Kuzmin[1,2], J. Adell[3], T. Balasubramian[3] and P. Laukkanen[1]
[1]Department of Physics and Astronomy, University of Turku, Finland
[2]Ioffe Physical-Technical Institute of the Russian Academy of Sciences, St. Petersburg 194021, Russian Federation
[3]Max-lab, Lund University, Sweden

4:30 – 4:50 PM O-16. **Growth and evolution of the native oxide on the atomically clean and $(NH_4)_2S$ treated $In_{0.53}Ga_{0.47}As$ surface**
B. Brennan[1], D. M. Zhernokletov[1], H. Dong[1], G. Hughes[2], and R. M. Wallace[1]
[1]Department of Material Science and Engineering, University of Texas at Dallas
[2]School of Physical Sciences, Dublin City University, Glasnevin, Ireland

4:50 – 5:10 PM O-17. **Advanced Nanostructures for Thermoelectric Energy Conversion**
Yue Wu[1]
[1]School of Chemical Engineering, Purdue University

5:10 – 6:40 PM **Poster Session** – **Galaxy Rooms (Student Union)**

6:40 – 9:00 PM **Picnic** – Student Union Mall and Reflection Pools (between Student Union and McDermott Library)

Tuesday, June 5, 2012

Session 1 Oral Presentations (Nottingham contestants) – Davidson Auditorium

7:30 – 8:30 AM Breakfast - JSOM Atrium

Moderator: *Daniel Dougherty, North Carolina State University*

8:30 – 8:50 AM N-01. **Quantum Tunneling Driven Assembly and Diffusion of Hydrogen and Deuterium on Cu(111)**
A.D. Jewell[1] and E.C.H. Sykes[1]
[1]Department of Chemistry, Tufts University

8:50 – 9:10 AM N-02. **Hydrogen interaction with Aluminum surfaces: Understanding hydrogenation / dehydrogenation reaction mechanisms in complex metal hydrides (alanates)**
I.S.Chopra[1] and Yves Chabal[2]
[1]Department of Physics and Astronomy, University of Texas at Dallas,
[2]Department of Material Science and Engineering, University of Texas at Dallas,

9:10 – 9:30 AM N-03. **Semiconductor Surfaces Directly Functionalized by Wet Chemistry Methods**
Fangyuan Tian[1], Andrew V. Teplyakov[1]
[1]Department of Chemistry & Biochemistry, University of Delaware

9:30 – 9:50 AM N-04. **Directing Self-Assembly of Nanostructures Kinetically and the Observation of Self-Limiting Growth of Mounds on Patterned GaAs(001)**
Chuan-Fu Lin[1] and R J Phaneuf[1]
[1]Department of Materials Science and Engineering and Laboratory of Physical Science, University of Maryland

9:50 – 10:10 AM **Morning Break – JSOM Atrium**

Session 2 Oral Presentations (Nottingham contestants) – Davidson Auditorium

Moderator: *Kyeong jae Cho, University of Texas at Dallas*

10:10 – 10:30 AM N-05. **Atomic Control of Freestanding Graphene with a Scanning Tunneling Microscope**
S. D. Barber[1] and P. M. Thibado[1]
[1]Department of Physics, University of Arkansas

10:30 – 10:50 AM N-06. **Molecular Interactions in Metal Organic Frameworks for Optimized Gas Separation, Storage and Sensing Applications**
N. Nijem[1] and Yves Chabal[1]
[1]Department of Materials Science and Engineering, University of Texas at Dallas

10:50 – 11:10 AM N-07. **Phase transformations and the direct visualization of the critical nucleus of BDA on Cu(001)**
D. Schwarz[1] and B. Poelsema[1]
[1]Physics of Interfaces and Nanomaterials, MESA+ Institute, University of Twente, The Netherlands

11:10 – 11:30 AM N-08. **Spin-exchange-induced dimerization of an atomic 1-D system**
N. Zaki[1] and R. M. Osgood[1,2]
[1]Department of Electrical Engineering, Columbia University, NY
[2]Department of Applied Physics, Columbia University

11:30 – 11:50 AM N-09. **Angle-Resolved Photoemission Studies of Topological Sb Thin Films**
Guang Bian[1], and Tai-Chang Chiang[2]
[1]Department of Physics, University of Illinois at Urbana-Champaign,
[2]Frederick Seitz Materials Research Laboratory, University of Illinois at Urbana-Champaign,

11:50 – 1:30 PM **Lunch Break – Galaxy Rooms (Student Union)**

Session 3 Invited and Oral Presentations (Nottingham contestants) – Davidson Auditorium

Moderator: *John Randall, Zyvex Laboratories Inc.*

1:30 – 2:10 PM **INVITED: Antenna-load interactions at optical frequencies: From impedance matching to quantum systems**
Robert L. Olmon[1] and Markus B. Raschke[1]
[1]Department of Physics, Department of Chemistry, and JILA, University of Colorado

2:10 – 2:30 PM N-10. **The Giant Surface Charge Density of Graphene Resolved From Scanning Tunneling Microscopy and First Principles Theory**
M.L. Ackerman[1] and P.M. Thibado[1]
[1]Department of Physics, University of Arkansas

2:30 – 2:50 PM N-11. **Growth of ZnO films on polar MgO(111) surfaces using atomic layer deposition**
K. Pradhan[1] and P. F. Lyman[1]
[1]Department of Physics and Laboratory for Surface Studies, University of Wisconsin-Milwaukee

2:50 – 3:10 PM N-12. **Multilayer Porphyrin Films via Copper(I)-Catalyzed Azide-Alkyne Cycloaddition: Film Properties and Applications in Dye-Sensitized Solar Cells**
P. K. B. Palomaki[1], P. H. Dinolfo[1]
[1]Department of Chemistry and Chemical Biology, Rensselaer Polytechnic Institute, St. Cogswell Laboratory

3:10 – 3:30 PM **Coffee Break – JSOM Atrium**

Session 4 Oral Presentations (Nottingham contestants) – Davidson Auditorium

Moderator: *Oliver Monti, University of Arizona*

3:30 – 3:50 PM N-13. **Layer-by-layer assembly of organic molecular donor-acceptor heterojunctions on vicinal gold surfaces**
Jun Wang[1] and Karsten Pohl[1]
[1]Department of Physics and Materials Science Program, University of New Hampshire

3:50 – 4:10 PM N-14. **The Metal to Non-metal Transition and Magnetic Properties in EuO:Gd**
Juan A. Colón Santana[1] and Peter A. Dowben[2]
[1]Department of Electrical Engineering, W. Scott Engineering Center,
[2]Department of Physics and Astronomy, Nebraska Center for Materials and Nanoscience, University of Nebraska-Lincoln

4:10 – 6:30 PM **Poster Session – Galaxy Rooms (Student Union)**

6:30 – 9:00 PM **Banquet** – Galaxy Rooms (Student Union)

Wednesday, June 6, 2012

Session 5 Oral Presentations – Davidson Auditorium

7:30 – 8:30 AM Breakfast - JSOM Atrium

Moderator: *Jason Slinker, University of Texas at Dallas*

8:30 – 8:50 AM O-18. **Passivation of the biosensor model surface system with 1-octadecenthiol**
Yue Liu[1] and Andrew V. Teplyakov[1]
[1]Department of Chemistry and Biochemistry, University of Delaware

8:50 – 9:10 AM O-19. **Multi-layer graphene films as electrodes for high performance of pentacene organic field effect transistors with surface treatments**
Sangchul Lee[1], Seok-Ju Kang[2], Gunho Jo[2], Yung Ho Kahng[3], Dong-Yu kim[2], Byoung Hun Lee[1,2] and Takhee Lee[4]
[1]Department of Nanobio Materials and Electronics, [2]School of Materials Science and Engineering, [3]Research Institute for Solar and Sustainable Energies Gwangju Institute of Science and Technology, Korea
[4]Department of Physics and Astronomy, Seoul National University, Korea

9:10 – 9:30 AM O-20. **Initial Studies of Precursor Environmentally Persistent Free Radical Adsorbates on Single-Crystal Oxide Surfaces**
M. C. Patterson[1], C. A. Thibodaux[2], R. L. Kurtz[1], E. D. Poliakoff[2], P. T. Sprunger[1]
[1]Department of Physics and Astronomy, Louisiana State University
[2]Department of Chemistry, Louisiana State University,

9:30 – 9:50 AM O-21. **Low-temperature Solution-processed Cadmium sulfide Thin-film Transistor and Its Stability**
A.L. Salas-Villasenor[1], I. Mejia, B. Gnade[1] and M. A. Quevedo-Lopez[1]
[1]Department of Materials Science and Engineering, University of Texas at Dallas

9:50 – 10:10 AM	**Morning Break – JSOM Atrium**

Session 6 Oral Presentations – Davidson Auditorium

Moderator: *Gary Kellogg, Sandia Laboratories*

10:10 – 10:30 AM	**O-22. Electrochemical and electronic properties of tetrahedral silicates Li_2MSiO_4 as cathode materials for Li-ion batteries** R. C. Longo[1], K. Xiong[1] and K. Cho[1] [1]Department of Materials Science & Engineering, University of Texas at Dallas
10:30 – 10:50 AM	O-23. **Real-time observations of ultra-thin iron oxide film growth on oxygen-deficient YSZ(001)** G. L. Kellogg[1] and Ivan Ermanoski[1] [1]Sandia National Laboratories
10:50 – 11:10 AM	O-24. **The Structure of the High Polarization Surface of the Antiferromagnet Cr_2O_3** Ning Wu[1], Xi He[1], Elio Vescovo[2], Wai-Ning Mei[3], Christian Binek[1], and Peter A. Dowben[1] [1]Department of Physics & Astronomy and the Nebraska Center for Materials and Nanoscience, University of Nebraska at Lincoln [2]Brookhaven National Laboratory, National Synchrotron Light Source [3]Department of Physics, University of Nebraska at Omaha,
11:10 – 11:30 AM	O-25. **Acceptor and surface states of ZnO nanocrystals: A unified model** S. T. Teklemichael[1] and M. D. McCluskey[1] [1]Department of Physics and Astronomy, Washington State University
11:30 – 1:00 PM	**Box Lunch** – JSOM Atrium
1:00 – 4:00 PM	**Tours of local industries** (Optional)
Thursday	**Meeting of the UT Dallas AVS Texas Chapter** (Optional)

O-01

Orientational Transition and Competitive Pathways in the Adsorption of Phenols on the Ge(100)-2 × 1 Surface

Bonggeun Shong and Stacey F. Bent

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Functionalization of semiconductor surfaces with organic molecules has been attracting increasing interest in recent years, in light of combining the tailorability of organics with semiconductor technology. Attachment of bifunctional molecules is especially interesting because of the possibilities for having one of the functionalities available for further modification. The (100) surfaces of Si or Ge form well-ordered arrays of reactive surface dimers after proper preparation in ultra-high vacuum. In this study, we compare reactions of phenol and hydroquinone (benzene-1,4-diol) on Ge(100)-2 × 1 by multiple internal reflection infrared (IR) spectroscopy, X-ray photoelectron spectroscopy (XPS), and density functional theory (DFT) calculations, and show that the dissociative adsorption of the second hydroxyl group in hydroquinone is prohibited by geometrical hindrance.

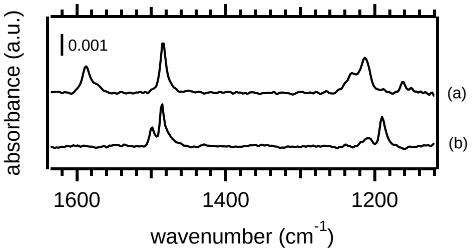

Fig. 1. FTIR spectra of (a) phenol, (b) hydroquinone chemisorbed on Ge(100)

First, phenol is adsorbed on Ge(100)-2 × 1 at 310 K [1]. IR spectra of chemisorbed phenol on Ge(100) match well with the calculated spectrum of O-H dissociated adsorbate. In DFT calculations, the activation barrier for the O-H dissociation is low enough to be overcome at 310 K, and the phenoxy adsorbate product is stable, supporting the assignment of the experimental result. Furthermore, a transition between two phenoxy adsorption configurations — lying down and standing up — is found as a function of phenol exposure.

In contrast, in the IR spectra of hydroquinone chemisorbed on Ge(100), blue-shifted minor peaks are discernible next to the major peaks [2]. The major peaks are assigned to dual dissociated hydroquinoxy adsorbate. The origin of the minor peaks can be deduced from the reaction pathway calculations. Although the first O-H dissociation barrier of hydroquinone is close to that of phenol, the second hydroxyl group encounters a much larger barrier for O-H dissociation once the molecule is attached to the surface. Furthermore, the second attachment is geometrically selective, determined by the distortion of the adsorbate molecule at each configuration. Therefore, a significant fraction of adsorbed hydroquinone cannot overcome the second activation barrier and remains in a singly-bound state, as confirmed by both XPS and IR, in which the blue-shifted peaks match the calculated IR spectrum of the singly-bound hydroquinoxy adsorbate.

References:

[1] B. Shong, and S. F. Bent, *J. Phys. Chem. C* (2012). DOI: 10.1021/jp3009767
[2] B. Shong, K. T. Wong, and S. F. Bent, *J. Phys. Chem. C* **116**, 4705 (2012)

O-02

The Picture Tells The Story:
STM Reveals The Mechanism of Silicon Oxidation

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Because of its immense technological importance, silicon oxidation has been studied intensely for decades; however, the disordered nature of the oxide makes these reactions notoriously difficult to understand. In this work, the oxidation reaction is coupled with a subsequent etching reaction, allowing oxidation to literally write an atomic-scale record of its reactivity into the etched surface — a record that can be decoded into site-specific reaction rates, and thus chemical understanding, with the aid of simulations and infrared spectroscopy. This record overturns the long-standing and much-applied mechanism for the aqueous oxidation of the technologically important face of silicon, Si(100), and shows that the unusually high reactivity of a previously unrecognized surface species leads to a self-propagating etching reaction and near-atomically-flat Si(100) surfaces. This finding shows that, contrary to expectation, the low-temperature oxidation of Si(100) is a highly site-specific reaction and suggests strategies for functionalization by low-temperature, solution-based reactions.

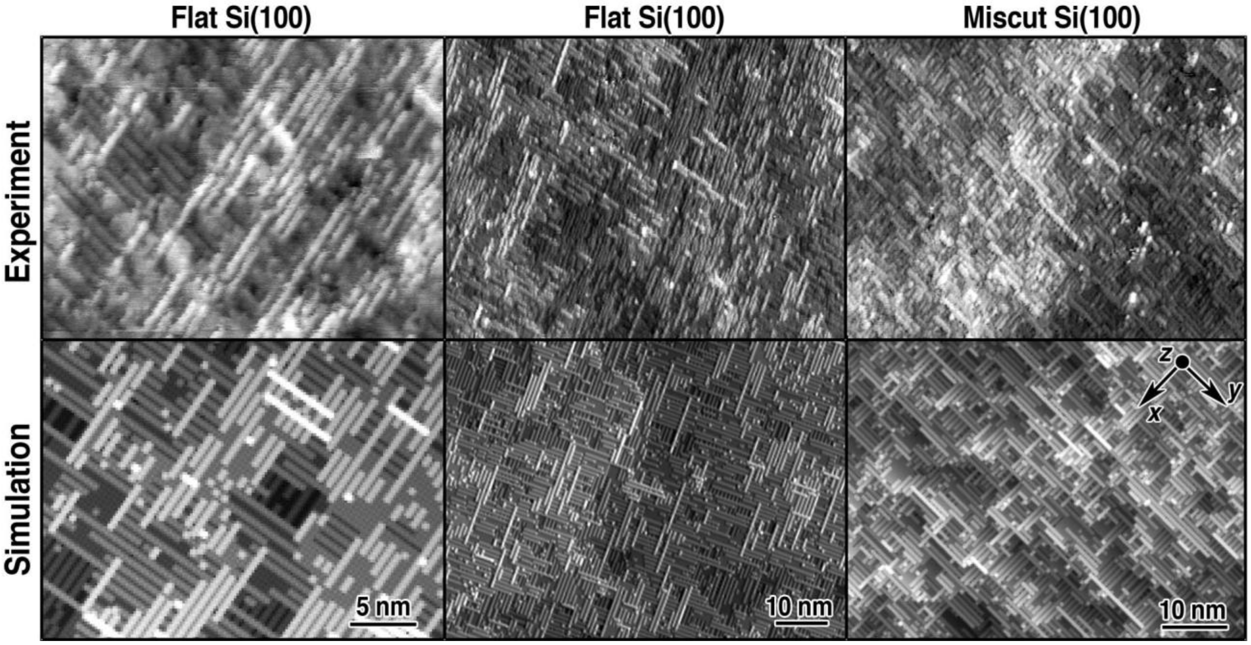

Fig. 1: STM images of flat and miscut NH_4F-etched Si(100) surfaces compared to kinetic Monte Carlo simulations of experimental images, rotated to match experimental orientations.

O-03

Activation of surface hydroxyl groups by modification of H-terminated Si(111) surfaces

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Wolf Gero Schmidt [2], **Kyeongjae Cho** [1] **and Yves J. Chabal** [1]

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Chemical functionalization of semiconductor surfaces, particularly silicon oxide, has enabled many technologically important applications (e.g. sensing, photovoltaics, and catalysis). For such processes, hydroxyl groups terminating the oxide surface constitute the primary reaction sites. However, their reactivity is often poor, hindering technologically important processes, such as surface phosphonation requiring a lengthy post-processing annealing step at 140°C with poor control of the bonding geometry. Using a novel oxide-free surface featuring a well-defined nanopatterned OH coverage, we demonstrate that hydroxyl groups on oxide-free silicon are more reactive than on silicon oxide. On this model surface, we show that a perfectly ordered layer of mono-dentate phosphonic acid molecules is chemically grafted *at room temperature* (see Figure 1) and explain why it remains completely stable in aqueous environments, in contrast to phosphonates grafted on silicon oxides. This fundamental understanding of chemical activity and surface stability suggests new directions to functionalize silicon for sensors, photovoltaic devices, and nanoelectronics.

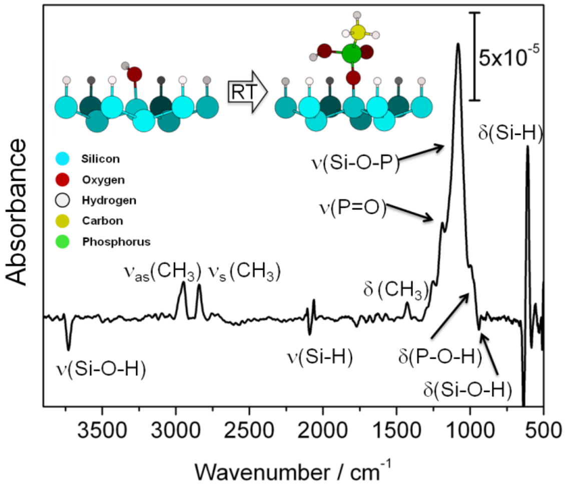

Figure 1: Differential infrared absorption spectrum: Transmission spectrum taken after the reaction with MPA (shown in inlet graph), referenced to the initial hydroxylated surface.

O-04

Reaction Pathways Involved Chemical Bath Deposition of Lead Sulfide on Functionalized Self-Assembled Monolayers

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We have investigated the reaction pathways involved in the chemical bath deposition (CBD) of lead sulfide (PbS) on –COOH, –OH, and –CH_3 terminated alkanethiolate self-assembled monolayers (SAMs) using time-of-flight second ion mass spectrometry (TOF SIMS), x-ray photoelectron spectroscopy (XPS), and scanning electron microscopy (SEM). This work has important applications in the development of photovoltaics, photodiodes and nonlinear optical devices.

CBD is a solution based method for the controlled deposition and semiconductor deposition.[1, 2] Using PbS CBD we demonstrate the selective growth and deposition of PbS films on functionalized SAMs. Two sizes of crystallites are observed to form: cubic nanoparticles and micron-sized crystallites. On –COOH terminated SAMs strongly adherent PbS nanocrystals form via an ion-by-ion reaction pathway. Initially, Pb^{2+} ions form complexes with the terminal carboxylate groups. The Pb^{2+}-carboxylate complexes then act as the nucleation sites for the ion-by-ion growth of PbS. In contrast, the micron-sized crystallites form in solution (cluster-by-cluster growth) and are observed on all SAMs studied. These crystallites can be easily removed from the surface using sonication. Thus under the appropriate experimental conditions PbS can be selectively deposited onto -COOH terminated SAMs. We illustrate this by selectively depositing PbS on a patterned -COOH/-CH_3 terminated SAM surface.

References:

[1] P. Lu, A.V. Walker, *ACS Nano*, **3** (2009) 370.

[2] P.Lu, Z. Shi, A.V.Walker, *Electrochimica Acta,* **55,**(2010), 8126-8134

O-05

High Quality Organic/Semiconductor Interface demonstrated by adding Al_2O_3 over the Organic Layer

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The electrical properties of organic/semiconductor interfaces are crucial for a variety of applications, such as organic transistors and organic/inorganic hybrid solar cells. However, the accurate characterization of these interfaces is prevented by the large tunneling current through the molecular layer[1], especially in the case of short chains. Moreover, standard fabrication methods, such as top metal contact via evaporation, cause damage during the processing even if applied directly with extreme caution. We present here a novel method to protect the interface with a layer of high-κ dielectric[2] (Al_2O_3) gently deposited on top of the organic layer using atomic layer deposition. The metal precursor reacts with the carboxylic head group of the self assembled monolayer (SAM) layer without affecting the underlying SAM/Si interface. Due to the increase of the dielectric layer thickness ($SAM+Al_2O_3$), a large reduction in tunneling leakage current occurs, and conductance voltage measurements can be implemented with a mercury probe setup. Moreover, the gate stack shows enough robustness to survive the entire MOS capacitor fabrication (i.e. metal evaporation). Capacitance voltage measurements show small frequency dispersion and a low D_{it}, on the order of 10^{11} $cm^{-2}eV^{-1}$, throughout the Si band gap for the intrinsic SAM/Si interface demonstrating inherent high quality when it is protected by the Al_2O_3 layer.

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[2] M. Li, M. Dai, and Y.J. Chabal, Langmuir 25 (4), 1911 (2009)

O-06

Effect of Oxygen on the Stability of Ag islands on Si(111)-(7x7)

Dahai Shao[1,2], **Xiaojie Liu**[1,3], **Ning Lu**[1,3], **C.-Z. Wang**[1,3], **Kai-Ming Ho**[1,3],
M.C. Tringides[1,3] **and P.A. Thiel**[1,2,4]

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We are working to determine whether an electronic effect known as the quantum size effect can influence chemisorption on Ag islands of different height, an effect which has been observed in some analogous systems such as O/Pb/Si. Therefore, we have used scanning tunneling microscopy to probe the effect of oxygen exposure on an ensemble of Ag islands separated by a Ag wetting layer on Si(111)-(7x7). Starting from a distribution dominated by islands that are 1 layer high (measured with respect to the wetting layer), coarsening in ultrahigh vacuum at room temperature leads to growth of 2-layer islands at the expense of 1-layer islands, which is expected. If, however, the sample is exposed to oxygen, coarsening leads to growth of 3-layer islands. There is no evidence for oxygen adsorption on top of Ag islands, but there is clear evidence for adsorption in the wetting layer. Density functional theory supports a model in which traces of oxygen on top of Ag islands can change the height-dependent relative stabilities of the islands. Therefore, in this system, the quantum size effect does not influence chemisorption. Instead, the reverse is true: chemisorption disrupts the quantum size effect and consequently changes the Ag island height distribution

O-07

Structure Evolution in Microaerosol-Deposited PCBM Monolayer Films on Au (111)

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Liquid deposition methods offer scalable low-cost routes to organic film growth and are increasingly employed in photovoltaic, microelectronic and display technologies. Active components, such as PCBM and polymers, can be dissolved in a solvent and delivered to the substrate via spin-coating, spray-jet, or wiper-blade methods depending upon application. Under such far-from-equilibrium growth conditions, resulting film morphologies are solvent sensitive and highly variable. Obtaining a molecular-level understanding of solute nucleation and growth and solvent expulsion is of fundamental interest and needed to advance liquid deposition technologies.

We have developed a liquid delivery sources with fine metering control to enable fundamental study of the deposition and growth of nonvolatile species. Micron-sized droplets are delivered to a sample substrate via a differentially pumped molecular beam source. In this quasi-supersonic source, trains of pulsed droplets impact the surface under UHV conditions. Single component films of [6, 6]-Phenyl-C_{61}-butyric acid methyl ester (PCBM), the most widely used electron-acceptor in organic photovoltaic devices, are generated from mM PBCM solutions. Nascent films, measured with UHV-STM, reveal glassy monolayers with substantial solvent incorporation. Subject to step-wise thermal annealing, PCBM monolayers exhibit two distinct crystalline domains, characterized by double-row and hexagonal-close-packed packing arrangements. The lower-density double-row phase was previously observed in films prepared by physical vapor deposition (PVD). The higher density hcp PCBM phase (Fig. 1) is newly observed and appears to be more thermodynamically favorable, but less kinetically accessible. Structural models for PCBM crystalline domains are presented, and supported by DFT computations. The extent of solvent retention under UHV conditions is remarkable and strongly impacts film structure evolution.

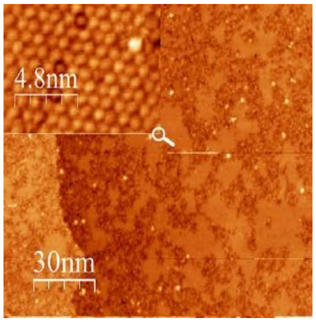

Figure 1. UHV-STM images of PCBM monolayer on Au (111) from pulsed microaerosol deposition and post annealing. Inset of hcp PCBM domains.

Nanophase separation of a PCBM-ZnPc binary mixture, also deposited with the microaerosol source, has been further explored. Upon growth and annealing of a 2ML mixture, PCBM and ZnPc undergo vertical phase separation, with ZnPc forming a well ordered monolayer in direct contact with Au (111) and PCBM segregating to the second layer. This separation reflects relative solubility, with the least soluble component (ZnPc) comprising the first deposited layer. This first-layer ZnPc film achieves a higher degree of ordering than ZnPc films prepared from single-component solutions, indicating stabilization by the terminating PCBM layer.

Acknowledgment: This work was supported by the NSF-MRSEC under DMR 0520471

O-08

Sub-monolayer Spin Rotation of Photoelectrons from FePC on Fe(110)

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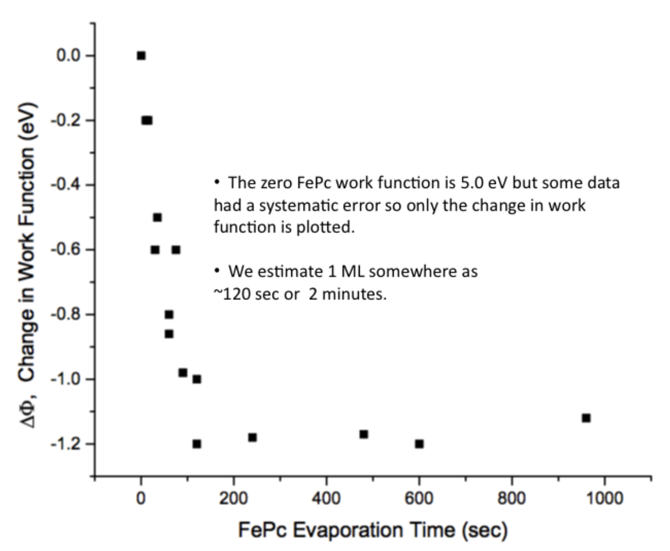
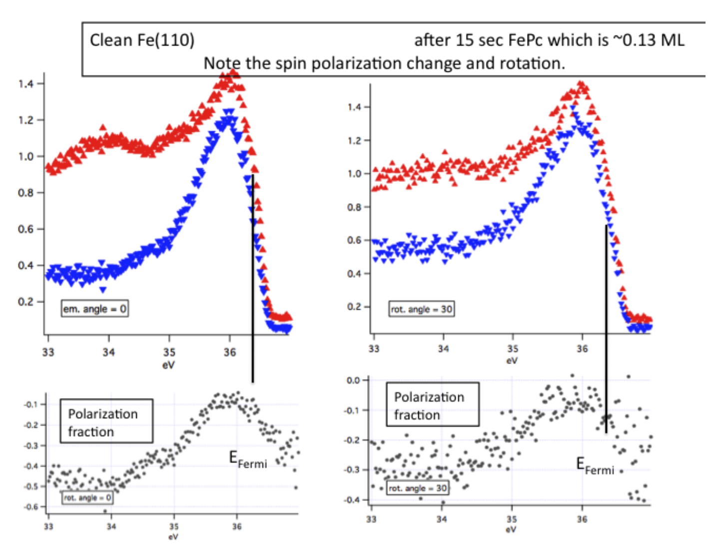
Spin-resolved photoemission at NSLS has been used to study the occupied electronic states of sub-monolayers to multi-layers of iron phthalocyanine (FePc) adsorbed on ~10-20 monolayer epitaxial films on Fe(110) on W(110). We find that the spin-resolved photoemission changes rapidly as a function of coverage and the initial (majority spin axis along [110] rotates by ~ 30 degrees for sub-monolayer coverage and then becomes unpolarized at ~1 monolayer (ML).

The coverage is determined by work function measurements as shown in Fig. 1. These were measurements from the low energy vacuum level cutoff of the bias sample using low intensity light to provide accurate intensity data.



- The zero FePc work function is 5.0 eV but some data had a systematic error so only the change in work function is plotted.
- We estimate 1 ML somewhere as ~120 sec or 2 minutes.

Fig. 1. Work function changes for FePc on Fe(110).



Clean Fe(110) after 15 sec FePc which is ~0.13 ML

Note the spin polarization change and rotation.

Fig. 2. Spin-resolved photoemission spectroscopy of FePc on

In Fig. 2 data are shown for clean Fe(110) showing highly polarized photoelectrons below the Fermi energy for B-field along [110} for majority-spin (red curves) and minority-spin (blue curves) electrons.

For 0.13 ML adsorbed FePc the spin polarization is somewhat reduced and is rotated from [110] towards [100] in the plane of the sample. We interpret this rotation as due to a strong coupling of the orbital moment of FePc with the metallic conduction electrons of the Fe substrate. At a coverage of ~0.25 ML the polarization is reduced to ~0 and then at higher coverage (~1 ML) it increases to about 1/2 of the inital polarization. These data suggest that molecular species are useful to modify the interface of spin-valve devices.

O-09

Hydrogen-Related Defects in Strontium Titanate

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Strontium titanate ($SrTiO_3$) is a perovskite oxide with unique structural and dielectric properties. It is a wide-band gap oxide semiconductor with indirect gap of 3.3 eV. It is one of the most useful single crystal substrates for electronic oxide thin film devices. $SrTiO_3$ thin films serve as building blocks for high-mobility oxide heterostructures that could lead to devices with superior operating characteristics.

Hydrogen is a ubiquitous impurity in oxide semiconductors and a potential source of n-type conductivity. Despite its prevalence, little is known about its behavior in $SrTiO_3$. Infrared (IR) absorption spectroscopy shows a hydrogen-related defect in $SrTiO_3$ with local vibrational modes (LVMs) at 3355 and 3384 cm^{-1} at liquid-helium temperatures. Isotope substitution experiments reveal that the defect consists of two hydrogen atoms bound to host oxygen atoms. Based on the temperature dependence of the LVMs and symmetry arguments, we propose that the defect contains a strontium vacancy passivated by two hydrogen atoms, where each hydrogen atom is bound to a nearest-neighbor oxygen atom and directed toward the strontium vacancy (Fig. 1). Preliminary results based on positron annihilation measurements suggest a correlation between vacancies and the LVMs. The thermal stability of the defect is determined through a series of isochronal annealing experiments on the hydrogenated $SrTiO_3$ sample. These measurements provide evidence of "hidden hydrogen," possibly H_2 molecules, in the crystal. Remarkably, in ZnO, a much less ionic crystal, hydrogen also passivates zinc vacancies [1] and form H_2 molecules [2,3]. It is therefore suggested that a "universal behavior" of hydrogen exists across a diverse range of oxides.

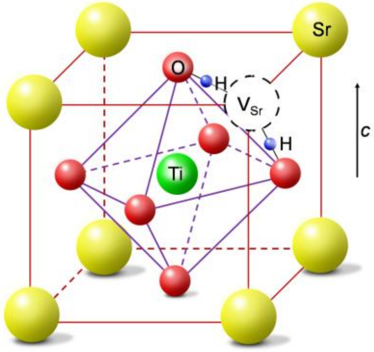

Fig. 1. Proposed model of hydrogen defect in $SrTiO_3$

The temperature dependence of the carrier density and mobility of an H-doped $SrTiO_3$ was investigated through Hall effect measurements. The carrier density shows an almost absence of carrier freeze-out, which may be attributed to the large dielectric constant of $SrTiO_3$, The Hall mobility is strongly temperature dependent, exhibiting a power-law dependence that suggests scattering of free carrier from optical phonons.

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[3] J S. Jokela and M.D. McCluskey, Phys. Rev. B **72**, 113201 (2005).

Invited

Electronic Structure and Excitations at Organic Semiconductor Interfaces

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Two-photon photoemission in combination with ultraviolet and x-ray photoemission and other surface science techniques is a powerful tool to study excitations and dynamics at interfaces. I will present recent results and applications of two-photon photoemission to study the excited state manifold and dynamics at the interface of organic semiconductors. Interfaces of complex π-conjugated organic molecules with metals offer a rich laboratory to investigate the interplay of band structure and localized molecular states. Effects of interfacial interactions are usually particularly prominent in the excited state manifold, offering an avenue to study under well-defined conditions the fundamental principles of interfacial charge-transfer [1].

Based on detailed studies of a class of organic semiconductors I will discuss how a simple model is capable of capturing the essence of the complex many-body physics governing the interfacial electronic structure in the weak coupling limit, making use of the intrinsic electrostatic moments of the organic semiconductor [2,3]. Such studies offer direct insight into the critical charge-transfer processes at interfaces of organic semiconductor-based structures used in solar energy conversion platforms such as organic photovoltaic cells.

References:

[1] Monti, O. L. A.; Steele, M. P. Influence of Electrostatic Fields on Molecular Electronic Structure: Insights for Interfacial Charge Transfer. *Phys. Chem. Chem. Phys.*, **12**, 12390–12400 (2010).

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O-10

Transition Metal Arenes for Graphene Molecular Doping

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There is considerable interest in controlling the doping concentration and doping type in graphene and in opening a band gap. Of the many approaches to doping graphene, molecular doping offers exceptional flexibility in that it depends on the chemistry of the doping molecule, which may be readily changed. In this vein, arene-metal complexes are particularly good candidates for molecular doping because either the metal atom or the arene group may be changed. For instance, interesting spin effects could be observed by changing the metal atom.

We started our exploration of molecular doping by depositing a Cr-benzene complex, in effect mimicking the well-known bis(benzene)chromium ($CrBz_2$) organometallic sandwich complex. Although calculations predict a stable graphene-Cr-benzene (G-Cr-Bz) complex with a strong binding energy, forming this complex in vacuum has been an experimental challenge. This difficulty may be due to a kinetic barrier preventing complex formation.

Our recent UHV STM and XPS results suggest the possible formation of G-Cr-Bz complex on graphene. The samples consisted of graphene CVD-grown on copper that had been transferred to a mica substrate. After annealing the sample in UHV at 380 K, the sample was cooled to 132 K and exposed to benzene to form an ice layer. Sub-monolayer Cr was then evaporated onto the benzene ice. All STM images and XPS data were collected at room temperature.

XPS and STM studies revealed that the benzene ice formed from a 40 L benzene exposure effectively prevented Cr deposition on the graphene surface. UPS and ELS data (obtained in complementary experiments using a HOPG substrate) show the formation of $CrBz_2$ for deposition on nominally "thick" layers of benzene ice. This species desorbs below room temperature and does not contribute to XPS or STM. For lower exposures, XPS showed that the surface Cr concentration increases with the inverse of the benzene exposure, indicating that not all the Cr reacts to form $CrBz_2$. STM images corroborate these results, showing an increase in the number and size of Cr clusters as the benzene exposure was decreased. After an 18 L benzene exposure, large areas of graphene and several Cr clusters are observed on the surface. Interestingly, as shown in Fig. 1, islands of small protrusions with one nm spacing can be found near the Cr clusters. We believe these protrusions to represent G-Cr-Bz complex islands.

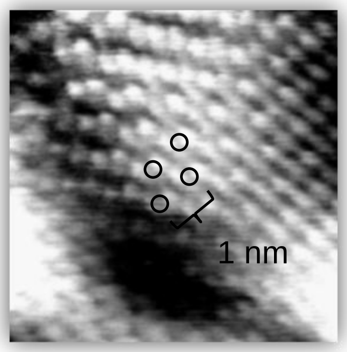

Fig. 1. STM image of possible G-Cr-Bz island on graphene. The open circles highlight the location of G-

O-11

Tunable Interface Electronic Properties at Metal-Graphene-Metal Sandwich Contacts

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Only a small fraction of all available metals has been used as electrode materials for carbon-based devices due to metal-graphene interface debonding problems. Those applicable metal electrodes (*e.g.*, Pd, Ti, Ni, Co, Cr), however, strongly interact with graphene, typified by substantial interface hybridization that may undermines the intrinsic structural and electronic properties of graphene.[1] We report an enhancement of the bonding energy of weakly interacting metals by using a metal-graphene-metal sandwich geometry, without sacrificing the intrinsic π-electron dispersions of graphene.[2] This sandwich structure further makes it possible to effectively tune the doping of graphene with an appropriate selection of metals. Density functional theory calculations reveal that the strengthening of the interface interaction is ascribed to an enhancement of interface dipole-dipole interactions. Raman scattering studies of metal-graphene-copper sandwiches are used to validate the theoretically predicted tuning of graphene doping through sandwich structures.

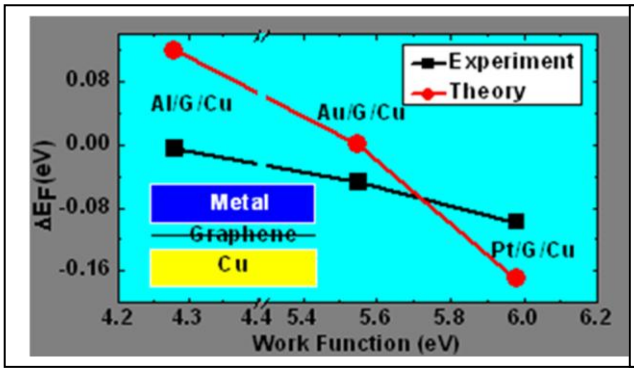

Fig. 1. Theoretical predictions and experimental evidence of the tunable doping of graphene in sandwich contacts. Inset is a schematic of metal/graphene/Cu sandwich structure.

References:

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[2] C. Gong, *et al.* ACS Nano (under review).

O-12

Low- κ organic layer as a top gate dielectric for graphene \ field effect transistors

G. Mordi[1], S. Jandhyala[2] and J. Kim[2]

[1]Department of Electrical Engineering, [2]Department of Materials Science and Engineering,
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Graphene, a two-dimensional (2D) hexagonal carbon lattice has been investigated as a conducting channel for field effect transistors (FETs) because of its exceptional properties, especially high mobility, high thermal stability, excellent mechanical and chemical properties. For graphene to be technologically viable, top gate dielectric deposition challenges have to be overcome which is due in part to a chemically inert basal plane.

Organic dielectrics are exciting materials because of their low-cost, low temperature applications and flexible features. Organic dielectrics can be suitable as gate dielectrics for graphene based flexible electronics if the dielectric is successfully scaled down to provide high enough capacitance and therefore good electrostatic control of the channel. It is reported that graphene-organic interface also shows improved quality due to fewer interface states and trap charges.[2,3] Particularly, parylene-C, a cross-linkable polymer with a hydrophobic surface has been widely investigated as a passivation layer[4] and even as gate dielectrics for flexible electronics and organic transistors

In this study, we deposit a thin layer of parylene C as the top gate dielectric for GFETs. These molecules are expected to noncovalently adhere to the graphene via π-π stacking and hydrophobic forces eliminating the need for functionalization as well as potential damage to the graphene layer or mobility degradation. Our results indicate good insulating properties from 7nm of parylene C with low trap density at the interface between the graphene and the parylene film.

We employ the Atomic force microscopy, Raman spectroscopy, X-ray photoelectron spectroscopy (XPS) and high resolution transmission electron microscope (HR-TEM) to characterize the dielectric. We will discuss in detail the electrical characteristics of our dual gated graphene field effect transistor (GFET)

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O-13

Potential Steps at Nanophase-Separated C_{60}-TiOPc-Ag(111) Interfaces

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Electric potential offsets at materials interfaces are used to direct charge transport and separation in organic electronic devices. Harnessing variations in the electric potential of nanostructured materials is key to improved performance. Spatially resolved measurements at well-defined molecular interfaces are needed to quantify local potential steps, and determine the extent that molecular orientation and interface dipole formation impact the electric potential landscape.

We report nanoscale structure – electric potential relations in monolayer films of the organic moleular semiconductors C_{60} and titanyl phthalocyanine (TiOPc) on Ag(111). Nanophase-separated monolayers were prepared under ultrahigh vacuum by physical vapor deposition and monitored with dual non-contact UHV- AFM and Scanned Kelvin Probe Miscroscopy (SKPM) for unambiguous mapping of molecular architecture and potential. The sensitivity and spatial resolution for potential measurement at a boundary were first established on Ag(111). On clean monatomic crystallographic steps, a 10 mV potential step (step-edge dipole = 1.4×10^{-3} e nm) reflects the electronic redistribution (*Smoluchowski* smoothing) about the step edge. Upon crossing the boundary between the neat Ag(111) surface and hexagonal close-paced C_{60} islands, a potential increase of □□=27±11 mV occurs. The local work function for C_{60} islands (□=4.77±0.01 eV) agrees quantitatively with monolayer-film values determined by photoemission.

The abrupt potential step across the hcp C_{60} – honeycomb TiOPc interface, □□= 207 ±66 mV, exhibits a 3.6 nm width that corresponds to the spatial resolution of our potential measurement across a boundary. The absence of banding in the SKPM image indicates a neligible (<0.012 e nm) lateral dipole per domain boundary molecule, with no evident charge redistribution. The potential step arises from work function differences between the local C_{60}/Ag(111) and TiOPc/Ag(111) monolayer domains, which are dominated by substrate interactions.

Acknowledgement: This work was supported by the NSF-MRSEC at the University of Maryland, DMR 0520471

O-14

Oxygen-induced (3×1) reconstruction on InAs(100) surface: Stable In-O-In subsurface trilayer

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Abstract It was recently found by us that oxygen induces ordered reconstructions on several III-V surfaces [1], which is significant, because ordered oxygen-induced reconstructions have not been reported to III-V semiconductor surfaces having zincblende structure. These reconstructions attract attention due to the immense interest in the development of oxide-semiconductor interfaces for the next generation metal-oxide-semiconductor-field-effect-transistors (MOSFETs). The formation of ordered oxides is attributed to significant stability of specific oxygen positions in the second surface layer, which is due to the exceptional surface structure of the $c(8\times2)$-ζ having III-V intermixed surface layer. The most oxygen-rich reconstruction shows (3×1) periodicity. A detailed atomic model is presented for this reconstruction in addition to the atomic model of the less oxygen-rich $c(4\times2)$ reconstruction. The uncommon (3×1) periodicity is attributed to the highly stable In-O-In trilayer below surface which also leads to significantly stabilizing additional bonds within the surface layer. The strain induced by the trilayer is more effectively accommodated within the (3×1) reconstruction than within the competing (2×1) reconstruction due to smaller number of dimers. It is proposed that the experimentally found semiconductivity is reached by substitutional atoms within the surface layer. The band gap of the (3x1) reconstruction with substitutional atoms in the surface layer is larger than that of the oxygen-induced $c(4\times2)$ reconstruction with 0.5 monolayers of oxygen, in agreement with the experimental results. It is deduced that the (3×1) reconstruction comprises about 1 monolayer of oxygen based on the electron counting rule and scanning-tunneling-microscopy images.

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O-15

Observation of Polar InN with Surface Fermi Level near Valence Band Maximum

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High electron concentrations of nominally undoped indium nitride (InN) films, in particular, a metallic *n*-accumulation layer at polar InN surfaces have hindered the development of InN films for high-efficiency solar cells and electronic devices. The previous measurements of polar InN have shown the Fermi level to locate at the conduction band minimum or above it.

By using scanning tunnelling microscopy/spectroscopy and high-resolution synchrotron-radiation photoemission we demonstrate the formation of polar InN, which has the Fermi level in the fundamental gap, near the valence band maximum, as predicted by recent calculations [1], on both Si(111) and GaN substrates.

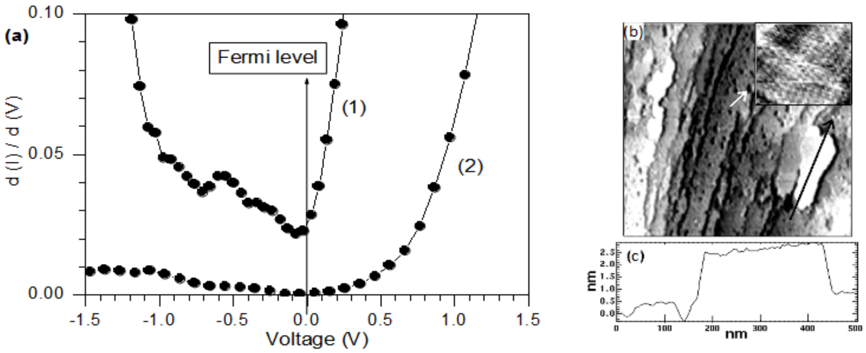

Fig 1. (a) Differentiated current-voltage curves from (1) Si(111)-In starting surface and from (2) the top surface of an InN island. (b) STM image from InN/Si(111) (c) Line profile along the black arrow in (b)

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O-16

Growth and evolution of the native oxide on the atomically clean and $(NH_4)_2S$ treated $In_{0.53}Ga_{0.47}As$ surface

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Due to the continued scaling of semiconductor devices, the incorporation of III-V semiconductor materials as the active channel material is predicted to be necessary to keep pace with expected performance. This is due to their inherent higher mobilities in comparison to silicon, which should lead to higher speeds and lower power consumption. InGaAs is one of the most promising candidate materials for this purpose, having a high electron mobility that scales with In content, and in the case of $In_{0.53}Ga_{0.47}As$, a sufficiently large band gap to ensure good device characteristics, as well as the added benefit of being lattice matched to InP, which can facilitate good material growth. These devices will also likely incorporate a high-k dielectric oxide layer, either in direct contact with the III-V channel or an alternative III-V barrier layer. Furthermore, the majority of oxide deposition processes involve some period of atmospheric exposure of the semiconductor, unless all deposition is carried out *in situ*; either after removal of a protective capping layer or immediately following the III-V growth. As a result, understanding the III-V/oxide interface is of critical importance, as the presence of interfacial oxide states have been shown to detrimentally impact device performance.

This study looks at the initial stages of native oxide growth on the oxide free $In_{0.53}Ga_{0.47}As$ surface, formed by removal of an arsenic cap *in* and exposing the sample to atmosphere for extended periods of time. growth of individual oxidation states [1] is then monitored u monochromatic X-ray photoelectron spectroscopy, after each indivi exposure. This is then compared to the oxide growth on an ammon sulfide ($(NH_4)_2S$) treated InGaAs sample. $(NH_4)_2S$ is typically used passivant to reduce the level of defect states present at the III-V/hig interface by decreasing interfacial oxidation and thereby restricting formation of arsenic dimers and dangling bonds.[2] The initial stage oxidation are seen to progress through formation of monovalent oxi which change over time forming more thermodynamically stable, As As_2O_5, Ga_2O_3 and In_2O_3 like states.

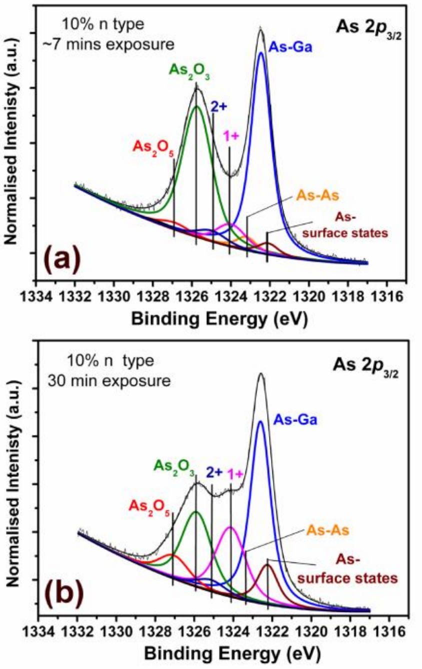

Fig 1. Change in As 2*p* peak after increased exposure to atmosphere.

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O-17

Advanced Nanostructures for Thermoelectric Energy Conversion

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Substantial efforts have been devoted to use nanostructured materials for thermoelectric energy harvesting and solid-state cooling in the past decade. However, the majority of the research is still limited in lab scale due to the incapability to mass-produce well-defined nanostructured materials with low yet industrial-compatible process. In addition, a lot of widely used thermoelectric materials contain toxic and expensive elements that prevent the large-scale deployment of the thermoelectric devices. In this presentation, we will discuss our research on the development of mass production of molecular scale nanostructures of chalcogenides and metal oxides, as well as their heterostructures, for the manufacture of thermoelectric generators operating at different temperature ranges. Particularly, we will talk about our approach to discover and investigate the non-toxic and abundant nanostructured materials to achieve an environmentally friendly process and the novel concept of flexible fiber-based thermoelectric design (highlighted by *Chemical & Engineering News*).

Our preliminary research indicated that thermoelectric figure of merit (ZT) larger than 2 could be achieved in the molecular scale nanowires of certain chalcogenide due to significantly enhanced power factor and reduced thermal conductivity as a result of quantum confinement.

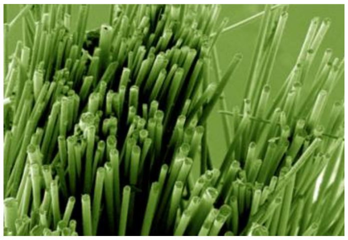

Fig. 1. A scanning electron microscopy image of flexible thermoelectric fibers.

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N01

Quantum Tunneling Driven Assembly and Diffusion of Hydrogen and Deuterium on Cu(111)

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Hydrogenation reactions are central to the petrochemical, fine chemical, pharmaceutical, and food industries and are of increasing interest in energy production and storage technologies. The processes of molecular adsorption, dissociation, diffusion, association, and desorption are important surface phenomena in heterogeneous catalysis. Typical heterogeneous catalysts often employ alloys based on platinum, palladium, rhodium and ruthenium. While these metals are active at modest temperature and pressure, they are not always 100% selective and are expensive.

Given that molecular hydrogen (H_2) dissociation is often the rate limiting step, one strategy is to engineer the minimal catalytic ensemble that will activate H_2 but leave the other reactants untouched. We describe a system which offers low dissociation barriers at one location on the surface and weaker binding in other regions. The Pd/Cu surface alloy was prepared in the dilute limit in which 1% Pd resides as individual, isolated substitutional atoms in a 99% Cu(111) surface. In terms of adsorption, these Pd atoms significantly lower the barrier to H_2 dissociation and allow the spillover of H atoms onto the Cu surface.[1]

This system also offers the opportunity to study the diffusion, association, and assembly of large quantities of H and D on the Cu(111) surface. Through careful low-temperature scanning tunneling microscopy (STM) tracking experiments we show that quantum tunneling effects dominate the diffusion properties of H and D on the Cu surface.[2] With this direct visualization and quantification of quantum tunneling effects in adatom diffusion, we reveal two types of weak interactions between H adatoms, which lead to assembly into small clusters and larger assemblies of small clusters. We show that the self-assembly of H into large islands is, in fact, a tunneling effect resulting from inter-atom energy being much smaller than the diffusion barrier. We further demonstrate that these latter effects are not at play for D. Density Functional Theory (DFT) calculations provide estimates for both diffusion and interaction energies. Theory also provides quantum tunneling probabilities that agree well with experiment.[2]

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N02

Hydrogen interaction with Aluminum surfaces: Understanding hydrogenation / dehydrogenation reaction mechanisms in complex metal hydrides (alanates)

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Hydrogen is considered as a fuel of the future. Among the various classes of materials currently considered, complex metal hydrides (alanates) have shown the most promise. The elementary reaction steps for hydrogen storage in the alanates have been broken up into molecular hydrogen dissociation on catalyzed aluminum, formation of alanes (mass transport) and finally the formation of complex metal hydrides. We have investigated the interaction of atomic hydrogen with single crystal Al surfaces to study the effect of crystal morphology and orientation on alane formation. Atomic hydrogen first impinges on step edges and with increasing hydrogen exposures forms alanes (AlH_3 1790cm^{-1}) on the step edges. As the atomic hydrogen exposures are further increased chemisorbed AlH_3 is physisorbed (1870cm^{-1}) and it oligomerizes to form high mass alanes (1910, 1724-1410cm^{-1}). Alane formation is enhanced on rough surfaces where the step density is higher. Al(100) surfaces have lower kinetics for alane formation due to higher barrier towards Al ad-atom, H atom and alane mobility.

We also demonstrate here that aluminum doped with very small amounts of Ti can activate molecular hydrogen at temperatures as low as 90K. The method is based on the ability to introduce a high flux of molecular hydrogen seeded with a guest molecule to probe the catalytic activity and H_2 dissociation. Once dissociated, hydrogen diffuses away from the catalytic site onto Al sites (i.e. spills over). We use this new method to determine the dependence of the catalytic activity of aluminum surfaces on Ti coverage (maximum for 0.1ML Ti coverage) and arrangement (next nearest neighbor catalytically most active).

We have also investigated the role of Titanium during the interaction of atomic hydrogen with Ti doped Al(111) surfaces and its effect on alane formation. Titanium is found to reduce the formation of large alanes, due to a decrease of hydrogen mobility and to trapping of small alanes on Ti sites thus hindering oligomerization. From the hydrogen storage perspective, the benefits of hydrogen activation by Ti containing catalytic sites on Al(111) is countered by the deleterious role of Ti in reducing mass transport through alane mobility and destabilizing high-mass alanes, which are two critical ingredients for the formation of complex metal hydride phases.

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N03

Semiconductor Surfaces Directly Functionalized by Wet Chemistry Methods

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We successfully attached NH_2-terminated SAM on silicon-on-insulator (SOI) (100) wafers with t-BOC protection group, and the X-ray photoelectron spectroscopy (XPS) measurements confirmed the Si-C bond formation and only one type of amine species presented on the surface. The high resolution cross-section transmission electron microscopy (TEM) image shows a neat SAM layer with apparent height of 1.7 nm, which was consistent with previous literature data and our density functional theory (DFT) calculations. This was also one of the first observed TEM images of a SAM on silicon. The second project was to investigate whether the use of t-BOC protecting group was necessary for primary amines during SAM modification process. Our DFT calculations show that if no protecting group was used, the structure was still expected to be thermodynamically favorable. We started conducting a series of experiments to explore the best scenario for growing NH_2-terminated SAM on Si(111) surfaces. So far, we have investigated different solvents to dilute pure 1-amino-10-undecene (AUD) compound as influenced by increased temperature, visible light and UV radiation. The results were also confirmed by atomic force microscopy (AFM) images and XPS spectra. Another project was to compare chemical and electronic properties of two traditional chemical preparation procedures for H-Si passivation: RCA and Piranha methods. It was found that the RCA cleaning method gave chemically uniform H-Si(111) surface with only mono-hydride present but shorter charge-carrier lifetime (meaning unsatisfactory electronic properties), while the Piranha method produced silicon surfaces with excellent electronic properties but not chemically well-ordered. We also conducted PCl_5 chlorination and SAM modification to compare these two methods. This work is fundamental for understanding silicon surface preparation and functionalization processes.

My most recent work focused on obtaining an –NH- termination on Si(111) surfaces through wet chemistry methods. We started from a well-ordered hydrogen-terminated Si(111) surface obtained from RCA cleaning method, then the H-Si(111) surface was chlorinated by PCl_5 to get Cl-Si(111) with every single silicon reactive site substituted by chlorine atom. After being treated with NH_3/THF solution for 1 hour at room temperature, the silicon surface was –NH- terminated. We confirmed this Si-NH-Si formation by IR, XPS, ToF-SIMS and DFT calculations. This is the simplest bench-top method so far to produce a stable silicon surface based on Si-N bonds. The experimental conditions are extremely mild: room temperature and no glove-box needed. Normally, the H-Si(111) and Cl-Si(111) surfaces are treated as general starting points for further surface modification, we believe that the newly characterized NH-Si(111) surface would definitely open a door for many potential applications.

N04

Directing Self-Assembly of Nanostructures Kinetically and the Observation of Self-Limiting Growth of Mounds on Patterned GaAs(001)

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A crucial issue in Materials Science is that of the stability of a moving interface. In the first part of this talk I describe an approach toward investigating this question, using lithographic patterning to perturb a flat crystalline surface over a range of spatial frequencies, followed by epitaxial growth. GaAs(001) shows a transient instability toward topographical perturbations. We model this behavior using and Ehrlich-Schwoebel (ES) barrier which impedes the diffusion of atoms across steps from above. We show via both kinetic Monte Carlo (kMC) simulations and molecular beam epitaxial (MBE) growth experiments that patterning in the presence of an ES barrier can be used to direct the self assembly of mounds [1].

Second, as we track the time evolution of mound formation, we find the evidence of "Self-Limiting Growth" on surfaces - we find that in the initial stage of growth, the pattern directs the spontaneous formation of multilayer islands at 2-fold bridge sites between neighboring nanopits along [110] crystal orientation, seemingly due to the presence of an Ehrlich-Schwoebel barrier and the effect of heterogeneous nucleation sites on the surfaces. However, as growth continues, the height of mounds at 2-fold bridge “self-limits”: the mounds cease to grow. Beyond this point an initially less favored 4-fold bridge site dominates and a different pattern of self assembled mounds begins [2]. The observation of self-limiting behavior brings us new understanding of mechanism for crystal growth. We also find that the transient amplification of pattern corrugation during growth is correlated with self-limiting behavior of mounds. We propose that a minimum, ‘critical terrace size’ at the top of each mound is responsible for the observed self-limiting growth behavior.

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N05

Atomic Control of Freestanding Graphene with a Scanning Tunneling Microscope

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Freestanding graphene has repeatedly demonstrated its superior quality when compared with graphene on a substrate. Furthermore, suspended graphene permits strain-induced distortions, dramatically changing the properties of the charge carriers. In this talk, an experimental approach is described to controllably and reversibly pull a freestanding graphene membrane any amount up to 35 nm from its equilibrium height by electrostatic manipulation with a scanning tunneling microscope (STM). In addition, STM images of freestanding graphene membranes with atomic resolution are presented and compared to STM images of graphene on copper. On suspended graphene, the atomic-scale corrugation amplitudes which were observed were 20 times larger than the STM electronic corrugation for graphene on a substrate. Both of these results are consequences of the freestanding graphene membrane behaving as a highly conductive yet flexible and elastic grounding plane, which responds to a local electrostatic attractive force created at the STM tip. These methods may potentially be applied in the controlled creation of pseudomagnetic fields by strain on single-layer graphene and to study the influence of local defects in suspended graphene membranes.

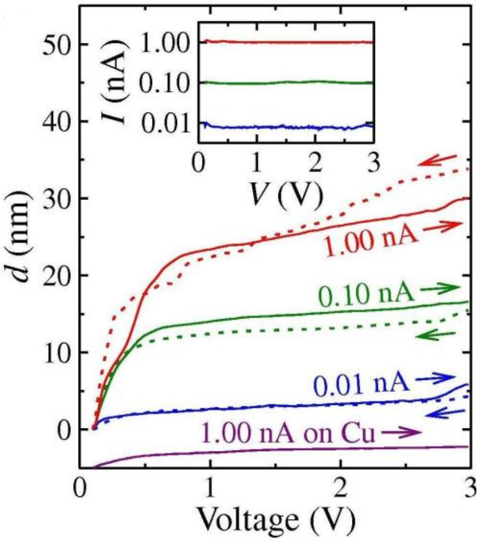

FIG. 1. Electrostatic manipulation STM data showing the vertical movement (*d*) of the STM tip vs. applied bias voltage for three different setpoint currents. The bottom trace is graphene on copper data that has been offset for clarity. Inset shows the measured current as a function of applied bias voltage.

This work is supported in part by the Office of Naval Research under Grant No. N00014-10-1-0181 and the National Science Foundation under Grant No. DMR-0855358.

N06

Molecular Interactions in Metal Organic Frameworks for Optimized Gas Separation, Storage and Sensing Applications

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Hydrogen storage and CO_2 capture are two of the most challenging problems for the development of renewable energy sources and the reduction of CO_2 emission. Hydrogen storage aims at storing a high volumetric density of hydrogen at room temperature. Fundamental studies exploring molecular hydrogen interactions in storage materials are therefore important to foster further development of materials. Metal-organic Frameworks are promising candidates for hydrogen storage and gas separation because their high surface area, porosity and structural tailorability all contribute to selective high hydrogen and CO_2 physisorption at specific sites in the structures.

This work explores the incorporation of hydrogen, CO_2 and hydrocarbons into various MOFs using infrared (IR) and Raman spectroscopy to characterize their interaction. IR spectroscopy can distinguish possible H_2 binding sites based on the perturbation of the initially IR inactive internal H_2 stretch mode. Comparative IR measurements are performed on MOFs with both saturated metal centers (e.g. M(bdc)(ted)$_{0.5}$) and unsaturated metal centers (e.g. MOF-74-M with M=Zn, Mg and Ni) by varying the ligand and/or the metal center. We combine room-temperature and high-pressure with low-temperature (20-100K) measurements and use theoretical van der Waals density functional (vdW-DF) calculations to derive quantitative information from the vibrational band shifts and dipole moment strengths.

In addition to H_2, we have explored CO_2 and hydrocarbon adsorption and selectivity in a flexible framework using Raman and IR spectroscopy. The CO_2 specific interaction with the framework and the specific connectivity of the metal to the ligands is key elements for this MOFs flexibility leading to its large CO_2 selectivity, and a novel adsorption behavior.

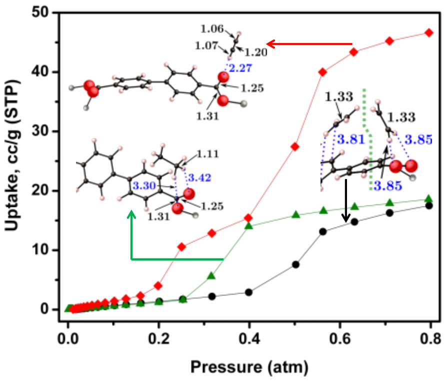

Fig.1. Adsorption isotherm of hydrocarbon C2 isomers, C_2H_2 (red), C_2H_3 (green) and C_2H_2 (black). Different gate opening pressures are

The unexpected gate opening behavior in this flexible framework upon the different hydrocarbon adsorption (Fig.1) is studied to uncover effects of specific hydrogen bonding on the gate opening characteristics. Identifying the specific interactions with the host leading to the desired and sought properties will guide the intelligent design for optimization of their gas separation and storage.

N07

Phase transformations and the direct visualization of the critical nucleus of BDA on Cu(001)

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We present a LEEM study of the growth of 4,4'-biphenyldicarboxylic-acid (BDA) on Cu(001) at temperatures between 300 K and 400 K. BDA is a linear molecule consisting of two phenyl rings with a carboxylic-acid group at opposite ends. During growth on Cu(001) the adsorbed BDA molecules form first a dilute phase. Once this phase reaches a sufficiently high density, a crystalline phase nucleates. In this phase the molecules form a hydrogen-bonded 2D supramolecular network with a c(8x8) superstructure [1,2]. By a careful analysis of the bright-field image intensity we can measure the density in the dilute phase, which is up to 40% of that in the crystalline phase. From the equilibrium densities at different temperatures we can construct the 2D phase diagram (see Fig. 1) and determine the 2D cohesive energy of BDA (0.35 eV).

During nucleation at low supersaturation, $\Delta\mu \approx 6$ meV, we observe critical behavior of huge clusters. The critical nucleus is found to be ≈ 600 nm^2. This result agrees nicely with that of classical nucleation theory using the supersaturation and the line tension derived from the cohesive energy. To our surprise, clusters being 4-6 times the critical nucleus still have a finite probability to decay and disappear during film growth.

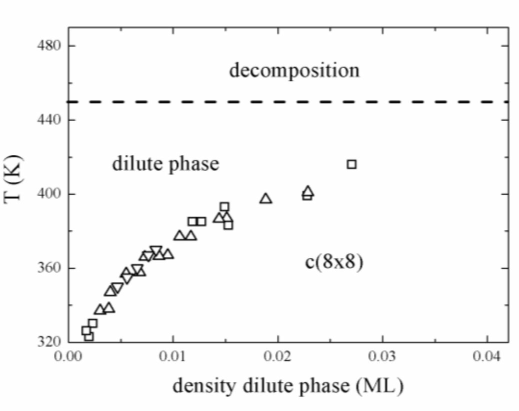

Fig. 1. 2D phase diagram for BDA on Cu(001). The data points show the equilibrium density in the diluted phase measured by analyzing the LEEM image intensity on the Cu terraces. BDA decomposes above 450 K on Cu.

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N08

Spin-exchange-induced dimerization of an atomic 1-D system

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True atomic systems when confined to one dimension exhibit a rich array of physical phenomena, simply because of the overriding rules of quantum mechanics for fermionic particles [1]. The predictions for such systems depend on the degree of electron correlations. One phenomenon that has been reported primarily for *s*-/*p*-orbital-derived heavy-metal single-atom-wide wires on semiconductor substrates is that of charge density wave (CDW) instabilities, in which the wires become insulating by way of a structural distortion [2]. Reasons given for this instability include classical Peierls distortion, Fermi nesting, and wire/substrate phonon interaction. However, the fundamental CDW instability driving mechanism for these atomic-wire systems is under debate. Here we show that Co (i.e. *d*-orbital-derived light metal) atomic wires on a *metallic* substrate can undergo a CDW instability based on spin-exchange interactions. By way of scanning tunneling microscopy (STM), we determine that the self-assembled wire array consists of dimerized atoms possessing a bond length that is 22% less than that of the underlying supporting vicinal substrate. We demonstrate that this relatively large distortion is due to the partially filled *d*-shell and a local high spin ferromagnetic ground state configuration of the wire atoms. The spin-exchange nature of this 1-D CDW instability has ramifications on its magnetic properties; we deduce its possible use as an atomic-scale spin-based binary memory element and raise its applicability to explaining break-junction experiment trends for magnetic metals.

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N09

Angle-Resolved Photoemission Studies of Topological Sb Thin Films

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Topological materials have unusual surface spin properties including a net surface spin current protected by the bulk symmetry properties. When such materials are reduced to thin films, their gapless spin-polarized surface states must connect, by analytic continuation, to bulk-derived quantum well states, which are spin-unpolarized in centrosymmetric systems. The nature of this passage in topologically nontrivial Sb films is investigated. Angle-resolved photoemission shows a smooth transition while calculations elucidate the correlated evolution of the spin and charge distributions in real space [1].

When the thickness of Sb films is further reduced to several atomic bilayers (BL), the Dirac states on the two faces of the film can overlap and couple by quantum tunneling, resulting in a thickness-dependent insulating gap at the Dirac point. Calculations for a freestanding Sb film with a thickness of four bilayers yield a gap of 36 meV (Fig. 1(c)), yet angle-resolved photoemission measurements of a film grown on Si(111) reveal no gap formation (Fig. 1(a)). The surprisingly robust Dirac cone is explained by calculations in terms of interfacial interaction [2].

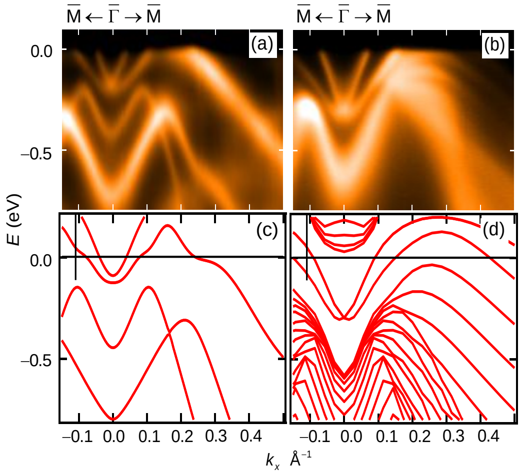

Fig. 1. (a, b) ARPES map for a 4-BL Sb film and a 20-BL Sb film taken along the $\bar{\Gamma}-\bar{M}$ direction. (c, d) Calculated band structure of 4-BL and 20-BL freestanding Sb films.

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Invited

Antenna-load interactions at optical frequencies: From impedance matching to quantum systems

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The goal of antenna design at optical frequencies is to deliver optical electromagnetic energy to loads in the form of, e.g., atoms, molecules, or semiconductor nano-structures, or to enhance the radiative emission from such structures, or both. A true optical antenna would, on a qualitatively new level, control the light-matter interaction on the nano-scale for controlled optical signal transduction, radiative decay engineering, quantum coherent control, super-resolution microscopy, and provide unprecedented sensitivity in spectroscopy. However, in contrast to the RF, where exact design rules for antennas, waveguides, and antenna-load matching in terms of their impedances are well established, substantial physical differences limit the simple extension of the RF concepts of antenna design to the optical regime.

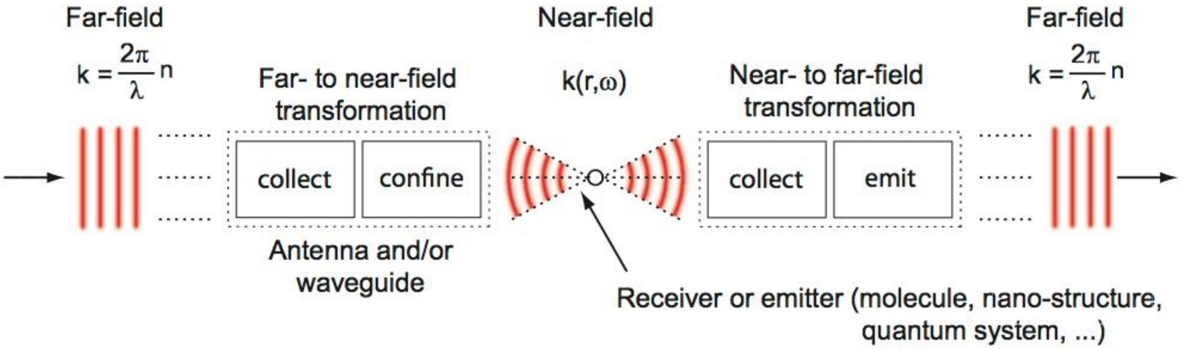

Fig. 1. Collection and confinement of propagating electromagnetic energy for delivery to a receiver or extraction for radiative emission from a source. A far-to-near-field transformation device optimizes the interaction between the propagating light and the nano-optical element. Similarly, light emission by a nano-optical device can be enhanced in terms of the radiative rate by using a near- to far-field transformer.

Here we generalize the ideal antenna-load interaction at optical frequencies, as illustrated in Fig. 1, characterized by far-field transformation from a propagating mode into an antenna resonance, the subsequent transformation of that mode into a nanoscale localization, and the free space transformation via an enhanced local density of states to a quantum load. These three steps define the goal of efficient transformation of incident radiation into a quantum excitation in an impedance matched fashion. We review the physical basis of the light-matter interaction at the transition from the rf to optical regime, discuss extension of antenna theory as needed for the design of impedance-matched optical antenna-load coupled systems, and provide several examples of the state of the art in design strategies and suggest future extensions. We furthermore suggest new measurable performance metrics based on electric vector field, measurement, field enhancement, and capture cross section to aid the comparison between different antenna designs.

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N10

The Giant Surface Charge Density of Graphene Resolved From Scanning Tunneling Microscopy and First Principles Theory

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Systematic constant-bias and variable-current measurements were made using scanning tunneling microscopy (STM) and first principles density functional theory (DFT) of graphene on a copper substrate. These measurements gave insight into the real-space electronic structure of the graphene, revealing that the graphene's charge density extends an unusually large distance from the nuclear plane. A comparison is made between the electronic density at the surface of graphene and graphite, revealing that the surface charge density of graphene is 300% that of graphite (Fig. 1). In addition, simulated STM images provide an explanation for the enhanced resolution obtained using high-current STM when imaging graphene.

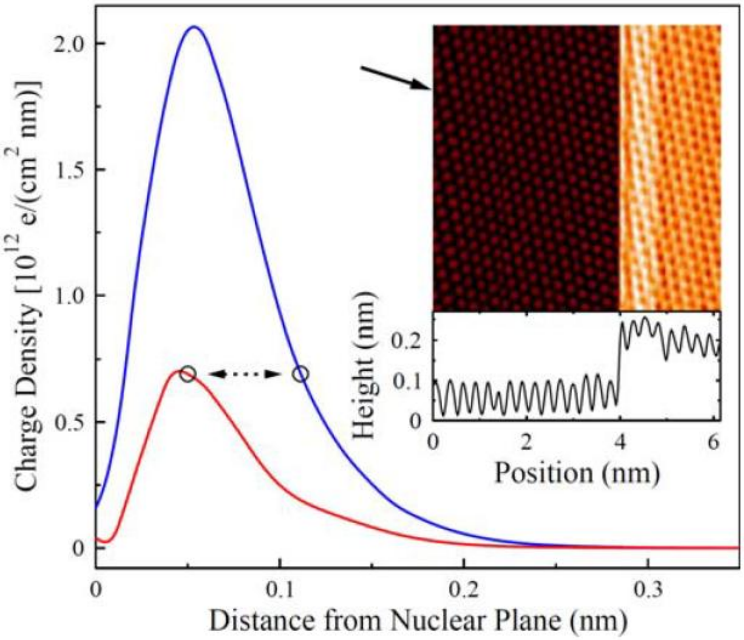

Fig. 1. Charge density of graphite (red) and graphene (blue) plotted as a function of distance from the nuclear plane. Inset: Experimental STM image of HOPG with an extracted line profile showing the height of the STM tip as a function of horizontal position. On the right is a section of graphene formed by spontaneous decoupling of the top layer of the HOPG. The line profile reveals the total retraction of the tip due to the increased surface charge density of the graphene.

N11

Growth of ZnO films on polar MgO(111) substrate using atomic layer deposition

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Polar hetrointerfaces of MgO(111) and II-VI semiconductor ZnO are of technological interest for transparent conducting electrode application. Growth and structure of thin films on polar surfaces can be different than on non-polar surfaces due to the large surface energy of polar surfaces. We have grown ZnO on unreconstructed (1x1)-OH terminated and reconstructed (√3x√3)R30^0 MgO(111) polar oxide surfaces using atomic layer deposition [1]. A homemade UHV-interfaced viscous-flow atomic layer deposition (ALD) reactor with *in-situ* quartz crystal monitor was used to grow ZnO thin films on the MgO(111) substrates [2]. In the ALD process temperature window, the growth rate was found to be ~2.3 Å/cycle. AFM revealed that the surface roughness increases with ZnO film thickness and that reconstructed MgO(111) is a better substrate for production of smooth ZnO films. XRD analysis revealed that ZnO thin films grown at 130$^{\circ 0}$C are polycrystalline, having the wurtzite structure, with preferential growth along the c-axis. ZnO grown on (√3x√3)R30^0 MgO(111) substrates show strong preferential growth along the (002) direction, whereas small amounts of growth along the (100) and (101) directions are also observed when grown on (1x1)-MgO(111) substrates. This indicates the crystal orientation during ALD ZnO growth not only depends on temperature but also on the surface terminations of the substrates.

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N12

Multilayer Porphyrin Films via Copper(I)-Catalyzed Azide-Alkyne Cycloaddition: Film Properties and Applications in Dye-Sensitized Solar Cells

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Solar energy may be the only renewable source of energy available to the human race that could provide the energy we require while at the same time minimizing negative impacts on the planet and population. In order for photovoltaic devices to succeed on a global scale, research and development must lead to reduced costs and/or increased efficiency. Dye-sensitized solar cells (DSSCs) are one class of next-generation photovoltaic technologies with the potential to realize these goals.

I will describe efforts towards developing a new light harvesting array of chromophores assembled on oxide substrates using copper(I)-catalyzed azide-alkyne cycloaddition (CuAAC) that could prove useful in improving DSCC performance. Specifically, molecular multilayers of porphyrin-based chromophores are fabricated via self-limiting CuAAC reactions to generate multilayered light harvesting films. Films of synthetic porphyrins, perylenes, and mixtures of the two are constructed in order to highlight the versatility of this molecular layer-by-layer (LbL) technique. Characterization in the form of electrochemical techniques, UV-Visible spectroscopy, infrared spectroscopy, water contact angle, and x-ray reflectivity all indicate that the films are reacting as expected.

Porphyrin light harvesting films assembled on ITO show a cathodic photocurrent when assembled in a DSSC device. Cobalt$^{3+/2+}$ and iodide/triiodide (I^-/I_3^-) redox mediators are commonly used in DSSCs as an electron shuttle. Devices operating with I^-/I_3^- show the largest photocurrents, but low open circuit potentials. Devices using cobalt$^{3+/2+}$ result in greater operating potentials than I^-/I_3^-. For all redox mediators tested, photocurrent increases with the addition of porphyrin layers beyond a monolayer. However, photocurrent reaches a maximum value at a point greater than one layer, after which it decreases. This demonstrates that multilayered porphyrin light harvesting films can be beneficial to improving DSSC performance but optimal film thickness (number of layers) is heavily dependent on the redox mediator. Electrochemical blocking layer studies suggest that the films could be useful as a self-passivating layer in DSSCs to reduce recombination effects and improve DSSC efficiency.

Our facile and versatile technique for creating molecular multilayer films may have implications in light harvesting materials, sensors, and molecular electronics. It could be amenable to large scale roll-to-roll processing which would be advantageous for applications requiring large surface area depositions.

N13

Layer-by-layer assembly of organic molecular donor-acceptor heterojunctions on vicinal gold surfaces

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Molecular co-self-assembly of organic electron-donor and electron-acceptor molecules into ordered heterostructures on surfaces provides a fundamental molecular-level insight into how these two kinds of molecules would interact in a model organic photovoltaic cell. We will present a study of precisely assembling the functionalized pentacenes (electron donors) and fullerenes (electron acceptors) into a layer-by-layer heterojunction on gold surfaces by scanning tunneling microscopy (STM) characterization and density functional theory (DFT) calculations (Fig. 1). The pentacene derivative --- 6,13-dichloropentacene (DCP) --- forms a striking long-range ordered brick-wall monolayer on a stepped Au(788) vicinal surface [1]. Subsequently deposited fullerene (C_{60}) molecules form parallel triple, double, and single long molecular chains on this intact DCP monolayer on Au(788) [2]. The novel organic-metal and organic-organic interfacial interactions have been explored and supported by DFT. These final structure formations are attributed to the delicate intermolecular Cl--H hydrogen bonding interactions, interfacial dipole fields and stepped-substrate-mediated interactions. The electronic properties for this model 3-component organic/metal system such as charge transfer between molecular donors and accepters have also been analyzed by DFT.

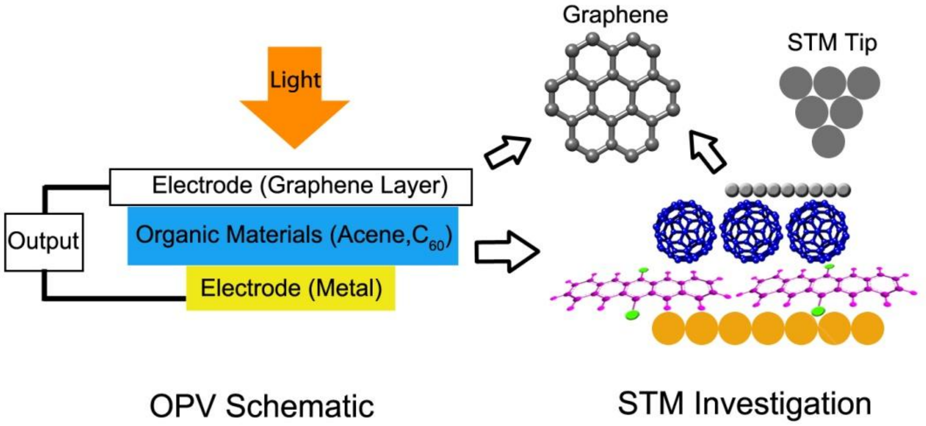

Fig. 1. A schematic for a model organic photovoltaic device composed of layer-by-layer advanced molecular materials (left) and a corresponding schematic representing a combined STM imaging and DFT modeling investigation for this system at a molecular level (right).

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N14

The Metal to Non-metal Transition and Magnetic Properties in the in EuO:Gd

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High quality films of EuO and $Eu_{0.096}Gd_{0.04}O$ were successfully grown on a p-type Si (100) substrate via pulsed laser deposition (PLD). X-ray diffraction (XRD) results show that the addition of Gd changes the growth texture orientation from [001] to [111] with both films crystallizing in the expected rock-salt structure [1]. Angular-resolved photoemission spectroscopy (ARPES) measurements confirms that doping EuO with Gd atoms has a strong influence in the electronic band structure of these films as well, revealing the presence of electron pockets around some of the high symmetry point in $Eu_{0.096}Gd_{0.04}O$ and $Eu_{0.096}Ce_{0.04}O$ films [2]. There is confirmation of the indirect nature of the EuO electronic band gap and suggesting a near semi-metallic character for the $Eu_{0.096}Gd_{0.04}O$ surface. Combined photoemission and inverse photoemission measurements suggests that under some circumstances that the surface appears p-type apparent rather than the expected n-type and this unexpected result is likely due to a reconstruction of the highly polar (111) surface. The combination of Gd doping and oxygen vacancies does lead to an appreciable density of states at the Fermi level and may be a contributing factor affecting the magnetic properties of these films [3]. We argue that this variability may be explained by band bending, which screens the electrostatic field of the polar surface.

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O-18

Passivation of the biosensor model surface system with 1-octadecenthiol

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One of the major issues encountered when designing biocompatible microelectronics surfaces is passivation of the reactive surface sites after the target sensing molecule has already been attached, so that the effect of the non-specific binding could be decreased. In this work, the biosensor model system is designed by using a single-strand biotin modified thiol DNA attached to the oxygen-free silicon substrate and streptavidin coated nanoparticles are used to test the reactivity of the surface. The binding of the biotin-modified thiol-DNA to the surface is performed through the sulfo-succinimidyl 4-(N-maleimidomethyl)-cyclohexane-1-carboxylate (SSMCC) crosslinker attached to an 11-amino-1-undecene self-assembled monolayer (SAM) on Si (111) surface. This designed surface is then reacted with streptavidin-coated gold nanoparticles, as summarized in Figure 1 below and the passivation of the reactive sites that remain on a surface is performed by 1-octadecenthiol (ODT). Atomic force microscopy and infrared and X-ray photoelectron spectroscopies are used to interrogate the structure of the interfaces produced, identity of the chemical functionalities, order of self-assembled layers, and the topography of the surface.

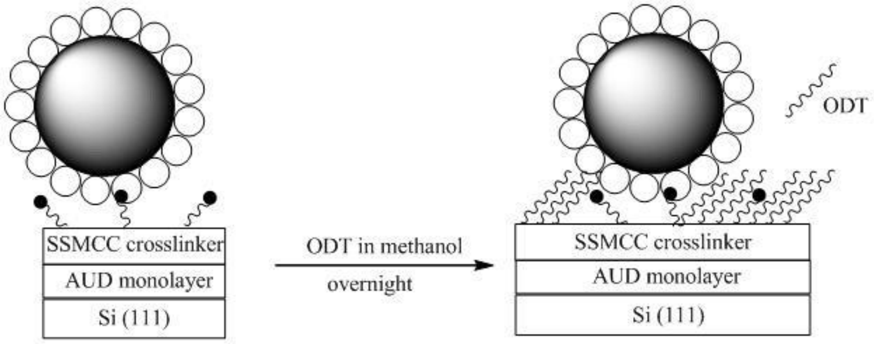

Figure 1. Schematic representation of the Si(111) surface modification scheme. According to the AFM studies of the nanoparticles deposited on a surface followed by passivation of the available surface reactive sites with ODT, the last step of modification resulted in 1 nm decrease of the apparent height of the nanoparticles. At the same time, the infrared spectroscopy suggests that the ODT forms a well-ordered SAM.

O-19

Multi-layer graphene films as electrodes for high performance of pentacene organic field effect transistors with surface treatments

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Organic field effect transistors (OFETs) have been attracting much attention due to their cost-efficient fabrication, limitless material variety, and the wide variety of potential applications [1]. In order to improve performance of OFETs, choosing appropriate contact electrode material and substrate treatments are significantly important [2,3].

Recently, graphene-based thin films have attracted a great deal of attention as an alternative electrode material. In particular, multilayer graphene electrodes have been found to have low contact resistance due to a lower charge-injection barrier to the pentacene active layer in OFETs compared with the traditional Au electrode, In addition, self-assembled-monolayer treatment for dielectrics, has been carried out in terms of decreased channel resistances and increased mobility.

In this presentation, we report on the highly improved performance of pentacene OFETs with graphene electrodes and surface treatments [2,3]. Detailed investigations revealed that performance improvement was induced from the formation of favorable interface which results in the reduction of the resistances.

Through detailed characterizations, the output and transfer currents were increased and the contact resistance was decreased. Moreover, we show significant improvement of OFET performances such as higher mobility of ~1.2 cm^2/Vsec. Our findings will foster establishing graphene-based thin films as an efficient electrode material for improving pentacene OFETs and other types of organic electronic devices.

This work was supported by the National Research Laboratory Program, a National Core Research Center grant, and the World Class University program from the Korean Ministry of Education, Science and Technology. This work was also partly supported by the core technology development program of the Research Institute for Solar and Sustainable Energies/GIST.

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O20

Initial Studies of Precursor Environmentally Persistent Free Radical Adsorbates on Single-Crystal Oxide Surfaces

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We report on the adsorption of phenol and 2-monochlorophenol (2-MCP) on metal oxide surfaces and nanoclusters in an effort to understand how environmentally persistent free radicals (EPFRs) are formed. EPFRs are known to form when aromatic hydrocarbon precursors are chemisorbed to metal oxide particles both under lab conditions [1] and in environmental sites [2]. The current study takes a surface science approach to study the atomic-scale formation of EPFRs on single-crystal alumina and TiO_2, as well as CuO nanoparticles, in order to guide a more fundamental understanding of the mechanism of radical formation. Electron paramagnetic resonance studies suggest EPFR formation is accompanied by a reduction of the metal oxide, as an electron is transferred to the substrate from the aromatic precursor [1, 2]. For the first time, we directly show through X-ray absorption near-edge spectroscopy (XANES) measurements that phenol-exposed CuO nanoparticles are reduced from Cu(II) oxide to a Cu(I) oxide species, with the smallest particles converted almost completely (98%) to Cu(I) oxide (see Fig. 1). In contrast, a bulk CuO standard showed no reduction after phenol exposure. Similarly, high-resolution X-ray photoelectron spectroscopy (XPS) measurements of single-crystal TiO_2 and thin-film Al_2O_3/NiAl(110) exposed to phenol and 2-MCP do not show evidence of metal reduction after adsorption of precursor molecules. Taken as a whole, these data imply that EPFR formation after precursor chemisorption may be correlated to the presence of available defect sites on the metal oxide, with radical formation only occurring at defects.

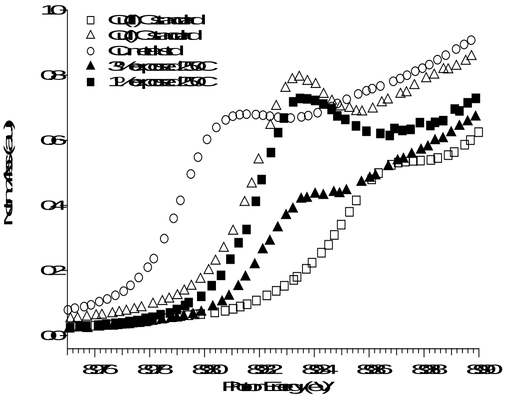

Fig. 1. XANES spectra of CuO nanoclusters on SiO_2 after exposure to phenol at 250°C. Smaller clusters (filled squares) are more completely reduced to Cu_2O than larger clusters (filled triangles).

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Research supported by the NIEHS Superfund Research Program grant 1P42ES013648-01A2.

O21

Low-temperature Solution-processed Cadmium sulfide Thin-film Transistor and Its Stability

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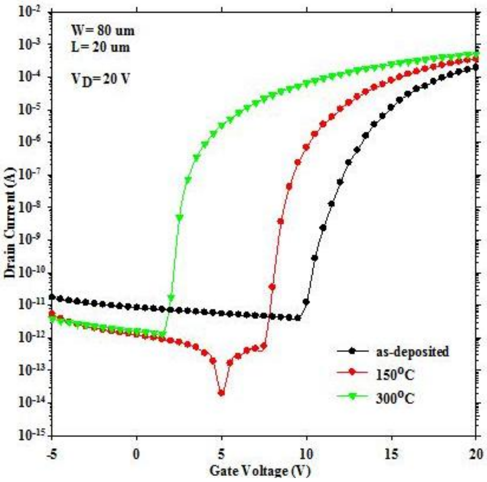
In recent years, fabrication of inexpensive electronics has become an increasing research area where both organic and inorganic materials are developed for simple and low-cost deposition techniques that will allow large-area flexible electronics. Among all, solution-processed deposition techniques, such as spin coating, inkjet printing and roll-to-roll printing, have the advantages of low cost and high throughput that have enabled printed electronics. Recently, some researchers have been reporting solution-processed high-performance CdS transistors from chemical bath deposition methods [1, 2]. However, there has been no research on the effect of the low-temperature annealing on the electrical properties and stability of CdS-based transistors.



In this work, we used CdS thin films as active layers. The CdS was deposited by chemical bath deposition from a $CdCl_2$ (cadmium chloride), $Na_3C_6H_5O_7$ (sodium citrate), KOH (potassium hydroxide), and $CS(NH_2)_2$ (thiourea) solution. The CdS films were deposited on HfO_2 gate dielectrics grown by ALD. Aluminum was used as source and drain contacts. Post-annealing was performed in Thermco MiniBrute atmospheric furnace system under forming gas atmosphere at 150°C and 300°C for one hour. All current voltage (I-V) characterizations of the CdS TFTs were carried out with a semiconductor parameter analyzer (Keithley 4200) in the dark at room temperature with V_D=20 V.

The effect of the annealing temperature of a solution-processed cadmium sulfide (CdS) thin-film transistor (TFT) was investigated. The characterization of CdS TFT improved with increasing annealing temperature. The active channel thickness was controlled to optimize the thin film transistor's properties. Good TFT properties were obtained at a relatively low thermal annealing temperature around 150°C and 300°C. The solution-processed CdS TFT showed mobility of ~20 cm^2/V s, an on-off ratio over 10^8, a threshold voltage that varies from ~15.5V, ~11.5V to ~3.2 V, for no anneal, 150°C and 300°C, respectively.

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O22

Electrochemical and electronic properties of tetrahedral silicates Li_2MSiO_4 as cathode materials for Li-ion batteries

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Using density functional theory (DFT), we investigate the structural, electronic and electrochemical properties of different tetrahedral silicate polymorphs recently synthesized and experimentally characterized. This family of compounds can insert and/or extract two Li atoms in two consecutive electron redox processes, giving rise to a much higher capacity (~330 mAh/g) than that of the current cathodes (e.g., ~160 mAh/g for $LiCoO_2$). Our DFT study includes the lithiated and both semi- and fully delithiated phases, in order to analyze how the charge/discharge process affects their structural stability. We also describe the electronic structure of these compounds accurately, trying to point out the main favorable mechanisms for both ionic and electronic conductivities. Finally, we show that, with suitable doping, it is possible to tailor the voltage and band gap of these silicates, improving their performance and making them promosing candidates as new cathode materials of rechargeable Li-ion batteries.

Acknowledgments

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O23

Real-time observations of ultra-thin iron oxide film growth on oxygen-deficient YSZ(001)

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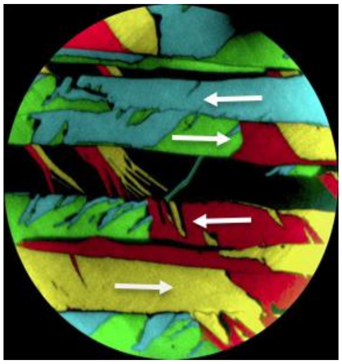
We use low energy electron microscopy (LEEM) and low energy electron diffraction (LEED) to study in real time the growth of iron oxide on the (001) surface of yttria-stabilized zirconia (YSZ). Investigations of the Fe_xO_y-YSZ system are motivated by its use as a working oxide for thermochemical fuel production via splitting of H_2O and CO_2 [1]. The films are grown by Fe deposition in a background of 10^{-6} to 10^{-5} Torr O_2 at temperatures of 1000°C and above. The first layer grows as FeO(111) with four non-equivalent domains arising from two rotational orientations and two stacking sequences (Fig. 1). Uniform spreading of 2-dimensional islands is observed by initiating growth at ~1000°C and raising the temperature to 1110-1145°C during Fe deposition. The growth is anisotropic with the fast growth direction depending strongly on both the rotational and stacking domain structure, most likely the result of preferred O_2 dissociation at specific island edge configurations. The FeO(111) film has a distinct LEEM-IV spectrum with three well-defined maxima and is easily distinguished from the YSZ(001) substrate. The coarsening of small islands (<10 nm diameter) at temperatures above 1160°C rotates the film orientation by 15° with respect to the substrate and reduces the coverage by about one half suggesting a dewetting process. Second-layer Fe oxide grows as $Fe_3O_4(111)$ and has a LEEM-IV fingerprint different from both FeO(111) and the YSZ(001) substrate.



composite of dark-field LEEM images showing four FeO(111) domains grown on YSZ(001). Arrows indicate preferred film growth direction.

This work was supported by the U. S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Science and Engineering and by the LDRD program at Sandia National Laboratories.

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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O24

The Structure of the High Polarization Surface of the Antiferromagnet Cr_2O_3

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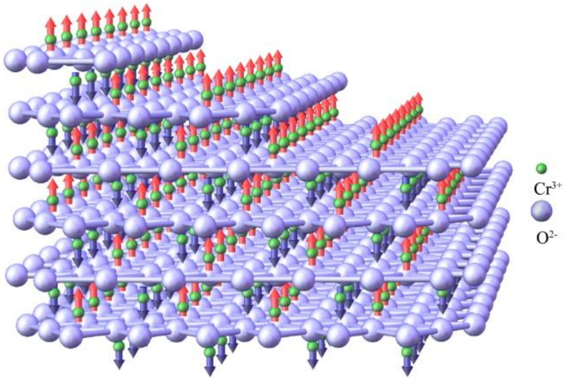

Fig. 1 The spin structure of a Cr_2O_3 single crystal with a stepped (0001) surface is shown for one of its two antiferromagnetic single-domain states. Up (red) and down (dark blue) spins of the Cr^{3+} ions (green spheres) point along the c

Manipulation of magnetically ordered states by electrical means is among the most promising approaches towards novel spintronic devices. Electric control of the exchange bias can be realized when the passive antiferromagnetic pinning layer is replaced by a magneto-electric antiferromagnet, like the prototypical magneto-electric Cr_2O_3(0001). Chromia works well in this case so long as there is also a finite remanent magnetization at the surface or boundary. We have demonstrated that a very unusual high polarization with magnetic order exists at the surface of the Cr_2O_3 (0001) and is robust against surface roughness from spin-polarized photoemission [1]. Both magnetic single domain and multi-domains were imaged by magnetic force microscopy and X-ray magnetic circular dichroism – photoemission electron microscopy (XMCD-PEEM) [2]. Using a ferromagnetic Pd/Co multilayer deposited on the (0001) surface of a Cr_2O_3 single crystal, we achieve reversible, room-temperature isothermal switching of the exchange-bias field, which reflects the switching of the bulk antiferromagnetic domain state and the interface boundary magnetization coupled to it [1]. We have also performed low energy electron diffraction LEED-I(V) analysis to explore the surface structure above and below Neel Temperature (308 K). Temperature dependent LEED was also carried out at several different electron kinetic energies and Debye temperature was extracted.

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O25

Acceptor and surface states of ZnO nanocrystals: A unified model

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Semiconductor nanocrystals have potential for a range of applications in optoelectronics and nonlinear optics. As the surface-to-volume ratio increases, surface emission processes become more important. Using IR and photoluminescence (PL) spectroscopy, we have developed a unified model for the acceptor and intragap surface states of ZnO nanocrystals. A PL peak, attributed to the transition of a free electron to the neutral acceptor, was observed at 2.97 eV. This observation is in agreement with an acceptor level previously observed in the IR [Teklemichael *et al.*, Appl. Phys. Lett. **98,** 232112 (2011)]. The temperature dependence of the IR absorption peaks, which correspond to a hole binding energy of 0.46 eV, showed an ionization activation energy of only 0.08 eV. The measured activation energy is attributed to thermal excitation of the hole from the acceptor ground state to a band of surface states 0.38 eV above the valence-band maximum. This model is in reasonable agreement with theoretical calculations that predict the existence of surface states 0.5 eV above the valence-band maximum. Therefore, while the acceptor is *deep* with respect to the bulk valence band, it is *shallow* with respect to surface states, raising the intriguing possibility of *p*-type surface conduction. A strong red PL emission centered at 1.84 eV is attributed to surface recombination. By monitoring the red emission band (at 650 nm) as a function of excitation energy, a photoluminescence excitation (PLE) spectrum was obtained, giving an onset at 3.0 eV. This feature is consistent with photon energies > 3.0 eV exciting electrons from the surface states to the conduction band, resulting in red emission after recombining with the holes. Photon energies < 3.0 eV excite electrons into the upper surface states, but with a reduced efficiency due to low density of states.

Poster Sessions

P01

Titanium Nitride as an Interface Material for Softening Neural Flexible Electronics

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Recording of extracellular neural activity and cell stimulation are key processes on the current and emerging technologies for neural prostheses and therapies. These are enabled by the use electrodes chronically interfaced with the nervous system [1]. One of the problems in the use of these electrodes is the large mechanical mismatch of the typically used probes, made of silicon micro needles or metal wires. The use of self-softening substrates for the fabrication of a new generation electrodes is of major interest to improve biocompatibility. A secondary problem is having a low impedance electrode and high injection capacity with safe reversibility [2]. These characteristics can potentially be achieved by the use of alternative materials such as TiN, IrO_x, and CNTs.

In this work Titanium Nitride electrodes are fabricated on a physiologically responsive substrate. Gold traces are used to improve signal to noise ratio of the device, and TiN pads interface with the electrolyte (Figure 1.a). Physical characterization has been performed on electrode pads prior and after cycling, presenting the relation of stoichiometry, crystalline structure and surface nanostructures (Figure 1.b) with Impedance and charge injection capacity.

Finding the optimum physical properties of the electrode pad material can lead to better implantable electrodes with low impedance and larger stimulation capacity.

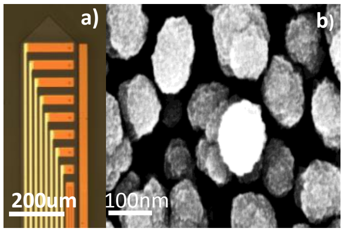

Fig. 1. a) Optical microscope image of Titanium nitride electrode fabricated on self-softening substrate. b) SEM image of TiN sputtered on polymer nanorods with the characteristic roughness of reactive plasma deposited films.

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P02

Softening Smart Polymers as Materials for Organic Thin Film Transistors for Neural Interfaces

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The increasing ability to ever more precisely identify and measure neural interactions and other phenomena in the central and peripheral nervous systems is revolutionizing our understanding of the human body and brain. To facilitate further understanding, more sophisticated neural devices, perhaps using microelectronics processing, must be fabricated. Materials often used in these devices, while suitable for these fabrication processes are not optimized for long-term use in the body and are often orders of magnitude stiffer than the tissue with which they interact. Using the smart polymer substrates described in this work, suitability for processing as well as chronic implantation is demonstrated. We explore how to integrate reliable circuitry onto these flexible, biocompatible substrates that can withstand the environment of the body. To increase the capabilities of these devices beyond individual channel sensing and stimulation, active electronics must be included into our systems. In order to add this functionality to these substrates and explore the limits of these devices, we developed a process to fabricate single organic thin film transistors with mobilities up to 0.1 cm^2/Vs and threshold voltages close to 0V. Also, to accomplish the long-term use of this technology we use smart polymer as an encapsulation layer, either by itself or combined with other inorganic materials such as Al_2O_3. This work will help with the understanding of fundamental problems for biocompatible, long-term electronic devices implants in the body, leading to a new set of tools and devices that will help understand problems in the neuroscience and materials research.

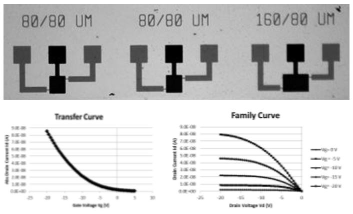

Fig. 1. Thin Film Transistors fabricated in softening smart polymer substrate and characteristic curves

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P03

A Path towards Single-Electron Devices

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As the minimum feature size in CMOS technology continues to decrease, quantum effects begin to dominate the operation of the transistors. In order to compensate for these effects, we require a new transistor design that operates based on the quantum effects present at the nanoscale. Single-electron transistors present a viable option to create smaller, more efficient transistors.

In addition to the increasing effect of quantum mechanics, current lithographic methods face challenges in scaling below the 10 - 20 nm scale. Several proposed lithographic methods, such as direct write methods, can provide high resolution lithography, enabling the creation of transistors in the sub-10 nm region. However, direct write methods require extensive development of multi-tip approaches to achieve throughput comparable to optical lithography.

A chemical method to fabricate devices can create high performance transistors with a high throughput. The first step of this process is the self-assembly of a monolayer of organic molecules on a hydrogen-passivated silicon surface. Second, mono-dispersed gold nanoparticles are deposited on the surface to form a tunnel junction. The electrical properties of the sample are determined by probing the surface with scanning tunneling microscopy (STM). This results in a double-tunnel junction. By properly tailoring the nanoparticle size, organic molecule size, and STM tip-sample distance, a Coulomb staircase can be observed in the I-V curve of the junction [1].

Using a 1.7 nm thick organic molecule, the beginning of a Coulomb staircase is observable one a small number of spectroscopy curves. However, the electronic response of each nanoparticle is not consistent. This suggests that thermal and electronic noise play a significant role in the measurement and behavior of double-tunnel junctions. By further optimizing the parameters of the surface, we hope create a more reliable electrical response in these double-tunnel junctions.

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P04

Highly Stretchable Thin Film Electrodes on Shape Memory Polymers

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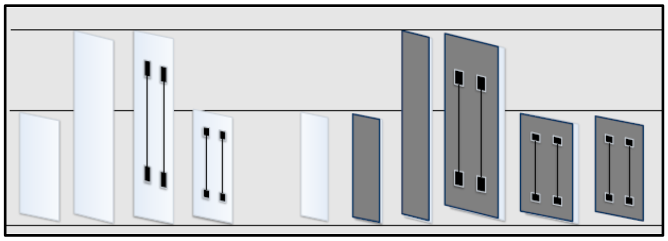

Fig. 1. SMPs serve as standalone electrode substrates (left) and can be used as carriers to pre-strain various elastomers before electrode

Stretchable and flexible electronics are utilized to fabricate a multitude of devices in today's world. Electronic circuits in a variety of these devices would be greatly benefitted if they possessed the ability to sustain large mechanical strain. Examples of such devices include multi-electrode arrays, cortical brain probes and cochlear implants. Shape memory polymers (SMPs) are a class of materials that provide a mechanical change in shape once activated by a stimulus. These materials can be temporarily configured by heating them through their glass transition temperature (T_g) to a rubbery state. To prepare the SMP substrate, methyl acrylate (MA) and isobornyl acrylate (IBoA) copolymers and bisphenol A ethoxylate di(meth)acrylate (BPAEDA) crosslinker were synthesized by free radical photo-polymerization using 2,2-dimethoxy-2-phenylacetophenone (DMPA) photoinitiator.

Two methods for processing flexible electronics based on tuning thermomechanical properties of SMPs have been explored. Within the first method, SMP substrates are synthesized and pre-strained between 0 and 50% at 10% intervals using a Universal Testing Machine to apply uniaxial strain. On top of these pre-strained SMPs, an E-beam evaporation process deposits a 3nm Ti adhesion layer before depositing a 30nm Au layer for the electrodes through a shadow mask. Samples are then heated above T_g enabling complete strain recovery while compressing and wrinkling the gold electrodes as shown in Figure 1. Before and after eliminating residual strain in the substrate, resistance measurements for the compressed electrodes are measured.

The SMP also can act as a carrier for poly(dimethylsiloxane) (PDMS) so that both polymers are strained together between 0 and 50% at intervals of 10%. Once the electrodes are deposited on the PDMS substrate, strain recovery is induced in either of two ways: heating the SMP above its glass transition temperature or peeling the PDMS from the SMP carrier. As in the first method, resistance measurements are conducted for the electrodes before and after strain release in the substrate. Moreover, wrinkling morphology in the electrodes on both the SMP and PDMS is characterized through SEM and AFM analysis. The results in this study are expected to greatly improve the strain capacity of current neural interfaces.

P05

CdS FinFET Based on 3D Simulation

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Abstract- Until today, Cadmium Sulfide (CdS) has been used for thin film transistors as the n-type device for use in flexible electronics [1]. In this paper we present for the first time a study of FinFETs with (CdS) film. We analyze the impact of important geometrical parameters of FinFETs devices, namely fin width (W_{FIN}) and fin high (H_{FIN}) [2]. All simulations were done in Atlas simulator where we use experimental parameters of CdS. In the sub-threshold region; subthreshold slope (S) and On-voltage were obtained and we can observe how the device can work like an enhancement or depletion mode as W_{FIN} change. Short-channel effects (SCE) of FinFET can be reasonably controlled by reducing either silicon fin height or fin width [3]. I_{ON}/I_{OFF} current is better due the better control of the current drive. Comparisons in total width between different transistors are done where thinness devices can make better use of its area.

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P06

Synthesis and Photoluminescence Switching in Alkyl Grafted Silicon Nanoparticles

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Photoluminescent silicon nanoparticles (Si NPs) have generated much interest due to their anticipated biocompatibility[1] and reasonably high visible quantum yield[2]. However, the synthesis of oxide-free Si NPs has proven difficult, and surface oxidation has been found to dramatically affect Si NP emission characteristics. Here, we report the synthesis and characterization of alkyl functionalized, red emitting photoluminescent (λ_{em}=590 nm) Si NPs for fluorescent marking applications. The 6-8 nm particles were characterized using FTIR and Raman spectroscopy and high resolution TEM. Changes in the emission characteristics of the Si NPs (e.g., emission intensity changes and observed emission color changes) were explored by subjecting the NPs to alcohols of varying chain lengths. The shift in photoluminescence (λ_{em}= 590 nm $\rightarrow$ λ_{em} = 430 nm), was highly dependent on the chain length of the alcohol. Subsequent FTIR experiments showed surface alkoxylation of the Si NPs after exposure to shortest straight chained alcohols. As the alcohol chain length increased; less access was available to unoccupied surface sites due to increased steric hindrance, this lessened the degree of surface alkoxylation and preserved the original emission color. These results indicate that blue emission is activated by alcohol passivation of surface defects, and that red emission results from the preservation of these defects.

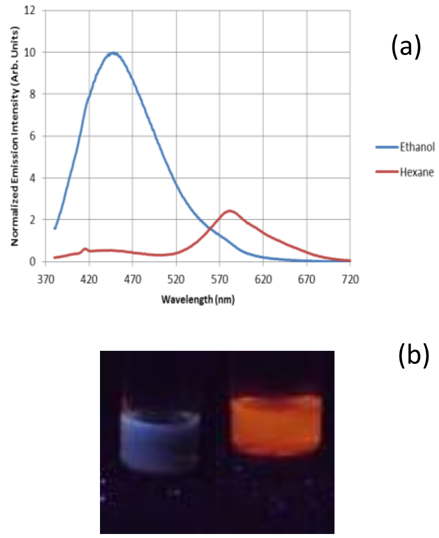

Fig. 1. (a) Emission profile of ethanolic dispersion of alkyl functionalized Si NPs (blue line) and hexane dispersion of Si NPs (red line)

(b) Corresponding fluorescence images of alkyl grafted silicon nanoparticles. On the left is an ethanolic dispersion of 1-decene functionalized Si NPs. On the right is a hexane dispersion of 1-decene functionalized Si NPs

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P07

In-situ interfacial study of e-beam Al deposition on native oxide InP (100)

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Metal Oxide Semiconductor (MOS) devices based on III-V semiconductor have attracted attention due to the potential higher mobility compared to that of Si based devices. However, the oxidation of the III-V / high-k interface can lead to Fermi-level pinning and frequency dispersion, which can strongly impact on electrical performance of III-V based devices [1, 2]. InP has been successfully used as a buffer layer between high-k oxides and III-V channel layers and achieved excellent electrical performance [3]. The interfacial quality of barrier layer and high-k dielectrics can strongly impact subthreshold swing and drain induced barrier lowering [4], so it is critical to understand the chemistry of the interface between InP and high k materials. Atomic Layer Deposition (ALD) "half cycle" studies of Al_2O_3 on the native oxide InP (100) surface using *in-situ* monochromatic X-ray Photoelectron Spectroscopy (XPS) has been reported [5]. The "clean up" effect whereby oxygen is seen to transfer from the native oxides to form Al_2O_3, was observed for In-oxides after the first pulse of trimethylaluminium (TMA), but the "clean up" effect did not occur for the P-oxides. In order to further remove the interfacial oxides, sacrificial metal Al can potentially be used to scavenge the oxygen from the In and P-oxides presented in the native oxide. In order to investigate this, a sequence of thin layer (on the order of monolayer) e-beam Al metal depositions were carried out on a native oxide InP (100) sample at room temperature. *In-situ* characterization is carried out using XPS, ultraviolet photoelectron spectroscopy (UPS), low energy helium ion spectroscopy (ISS) and reflective high energy electron diffraction (RHEED), after each successive deposition, in order to understand the detailed evolution of the interfacial oxides during the deposition.

This work is supported by the Semiconductor Research Corporation FCRP MSD Focus Center, the Nanoelectronics Research Initiative and the National Institute of Standards and Technology through the Midwest Institute for Nanoelectronics Discovery (MIND) and the NSF (ECCS-0925844).

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P08

In situ Raman and FTIR Study of the Thermal Effect on Graphene Transferred to SiO$_2$

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Thermal annealing is widely used to remove the PMMA residues on transferred graphene and the intercalated water at the graphene/SiO$_2$ interface.[1] Recent experimental progress shows that both the doping behavior and the carrier mobility in the transferred graphene undergo a transition at ~200℃ annealing.[2] In this work, we applied *in-situ* Raman and Fourier transform infrared spectroscopy (FTIR) study of the thermal effect on the transferred graphene on SiO$_2$ substrates. The Raman results show the same transition as reported in the previous literature.[2] The FTIR results imply that the decomposition of PMMA and the removal of the interface H$_2$O contribute to the reduced p-type doping behavior of graphene after below 200℃ annealing, but the close contact with SiO$_2$ surface (terminated by hydroxyl groups) contributes to the increased p-type doping and the degraded carrier mobility in graphene after above 200℃ annealing.

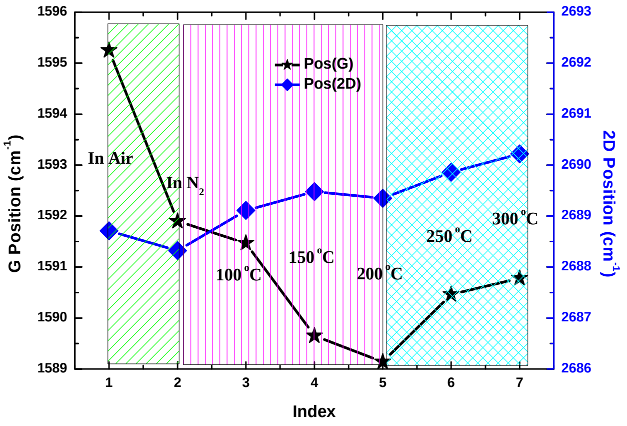

Fig. 1. *In-situ* Raman characterization of the thermal effect of transferred graphene on SiO$_2$ substrate.

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P09

New Possibilities in Low Energy Ion Scattering (LEIS) for Thin Film Analysis

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Low Energy Ion Scattering (LEIS) has been used for elemental characterization of surfaces already for many years. However, to make use of its unique surface sensitivity and quantitative nature, sample damage induced by the primary ion beam during analysis has to be avoided. Since the development of dedicated high sensitivity and high resolution analyzers [1], the required ion dose has become low enough to work under so called "static" conditions. LEIS is used for a variety of analytical applications where the elemental composition of the outermost atomic layer is of interest, from polymers to catalysts to thin films.

In LEIS, the surface is bombarded with 1 - 10 keV noble gas ions. Energy spectroscopy of the backscattered ions allows the surface atom involved in each scattering event to be identified. Quantification of the surface coverage is possible by comparison with reference samples. Due to strong neutralization of the primary ions before scattering at deeper layers, the information is primarily specific to the outermost atomic layer. Furthermore, scattering at deeper layers in combination with additional depth dependent energy losses yield a concentration profile of the first few nm of the sample.

In this contribution, we demonstrate the new possibilities of the technique in thin film analysis. This includes analysis of laterally structured samples applying a new generation of ion sources, which significantly improves the lateral resolution. Also, a comparison with other techniques like MEIS and TOF-SIMS is performed, using As implants in Si as test samples in a depth range of a few nm. First results are comparable to MEIS data, but with the advantage of simple and compact instrumentation. Compared to sputtering techniques like TOF-SIMS, quantification is simplified as sputtering induced effects do not occur.

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P10

Study of Transparent Zinc Oxide Thin-Films Transistors Deposited by Pulsed Laser Deposition

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In this work we demonstrate transparent thin film transistor using zinc oxide (ZnO) films as the semiconductor. ZnO films were studied as function of PLD deposition conditions such as O_2 pressure, substrate temperature, thickness, and laser energy. Materials analysis to demonstrate that oxygen partial pressure during deposition of the ZnO films is critical to achieve device quality ZnO films.

Full photolithographic process on glass substrate is reported. For the transparent TFTs, PLD-deposited Al_2O_3:ZnO (AZO) is used as gate, source and drain contacts. Figure 1 show the resulting transparent ZnO TFTs fabricated on glass. Resulting devices show transmittance of about 80%. Figure 2 show the electrical behavior of the transparent ZnO TFT with carrier mobilities >10 cm^2/V-s, a threshold voltage below 7 V and an I_{ON}/I_{OFF} ratio of $5x10^6$ were achieved.

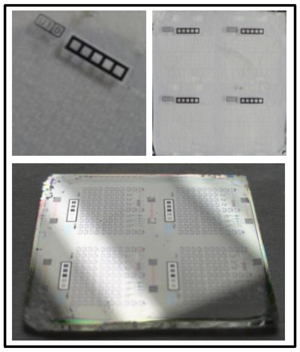

Figure 1. Transparent ZnO TFTs on glass substrate.

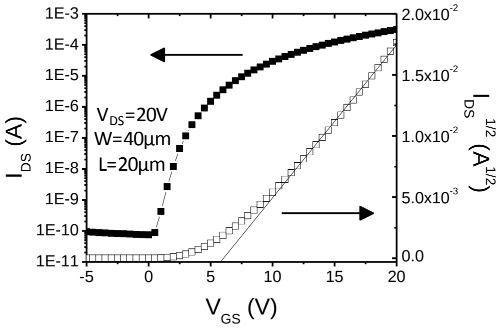

Figure 2. Transparent ZnO TFT electrical behavior (I_D-V_{GS}) at V_{DS}=20V.

P11

Properties of transparent conducting aluminum-doped zinc oxide films grown by RF-magnetron sputtering and pulsed laser deposition.

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Aluminum-doped zinc oxide (AZO) was deposited by RF magnetron sputtering and Pulsed Laser Deposition (PLD). Structural, electrical and optical properties were analyzed as a function of deposition conditions. Resistivity of the films was measured by four-point probe and Hall Effect, obtaining values below $9x10^{-4}$ Ω-cm for specific deposition conditions in both systems. The optical transmittance was measured in the 300-1000 nm wavelength range and the optical band-gap was determined, varying from 3.50 to 3.67 eV. Fig.1 shows the difference between the PLD and sputtering in terms of transparency and structure for 100 nm thick films. In Fig.1 the sheet resistance is 90 and 177 ohm/square for the PLD and sputtering films, respectively. Sputtering films are more polycrystalline and transparent. In the other hand, PLD films are preferred oriented in the (002) plane with lower transmittance but lower resistivity. The transparent and conductive AZO films developed in this work are promising candidates for their use as transparent electrodes in solar cells and thin film transistor for flexible electronics applications.

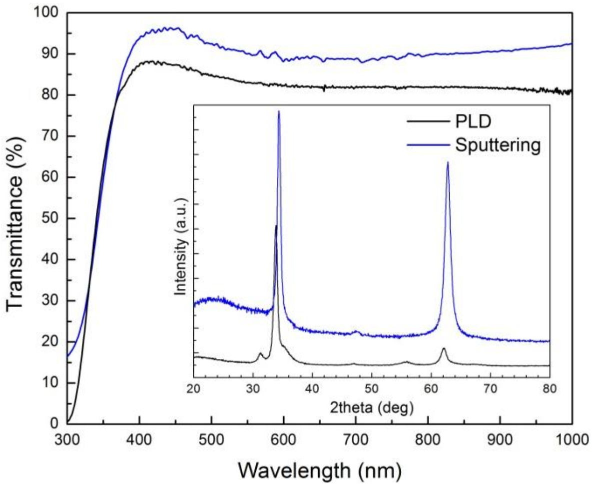

Fig. 1 UV-Vis transmittance and XRD patterns for 100 nm thick PLD and Sputtering films.

P12

Deposition of organic-inorganic-hybrid thin films using ozone based molecular layer deposition (MLD)

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Recently, organic thin films have been attracting attentions due to their flexibility and transparency which are suitable for large-scale display and flexible electronics applications. Alternatively, inorganic thin films have several benefits over organic thin films such as high functionality (e.g. high conductance, high dielectric constant or high polarization, etc.) Organic-inorganic hybridization is interesting because it can widen the range of their applications with new functionalities.

A novel technique has been reported using a modified atomic layer deposition (ALD) method, named molecular layer deposition (MLD) [1,2], which can be applied to build an organic and inorganic hybrid stack [3,4]. Hybrid thin films by MLD minimized the formation of defects during the growth of the organic and inorganic layers because they are deposited by sequential, self-limiting surface reactions similar to ALD process.

In this study, we investigated the growth characteristics of organic-inorganic laminates, i.e. 7-octenytrichlorosilane (7-OTS) and metal-oxide hybrid thin film, using ozone based MLD. 7-OTS is deposited by an exchanging reaction between functional group and water with growth rate of ~0.6 nm per cycle. The terminal vinyl group (C=C) of 7-OTS is converted into a carboxylic group (-COOH) through in-situ ozone (O_3) modification. Metal oxide is then deposited as a linker layer in-between each OTS layers using conventional ALD precursors, such as trimethyl aluminium (TMA), titanium tetrachloride ($TiCl_4$), diethyl zinc (DEZ) and water. Effect of temperature, dosing time and UV activation will be discussed.

Characterization of organic-inorganic hybrid thin films have been extensively investigated using transmission electron microscopy (TEM), scanning electron microscopy (SEM), atomic force microscopy (AFM), X-ray diffraction (XRD), and Fourier transform infrared spectroscopy (FTIR).

This research is partially funded through Korea-US collaboration R/D program by MKE-COSAR-KETI.

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P13

Understanding the Interaction of Atomic Layer Deposition (ALD) Precursors on Graphene

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In order to realize high-performance graphene based field-effect devices, one of the primary requirements is to be able to deposit high-quality, scalable high-κ dielectrics on graphene without degrading its properties [1]. Atomic layer deposition (ALD) is an ideal technique for achieving such dielectrics because of the ability to precisely control thickness and conformally deposit materials. However, ALD is a surface-reaction limited process [2] and graphene, being sp^2 bonded, has no out-of-plane covalent functional groups [3] and this can cause difficulties in initiating the ALD reaction [4]. In previous studies we have shown that using a reversibly physisorbed ozone (O_3) functionalization approach, we can deposit high quality ALD oxides (such as Al_2O_3) on graphene with thicknesses < 5 nm [5]. Further understanding regarding the interaction of oxidants and metal precursors with graphene is required for successfully applying ALD processes to deposit different oxides.

In this study, we will use *in-situ* electrical measurements of graphene devices inside an ALD chamber as a characterization technique in order to understand the adhesion mechanisms of oxidants (such as O_3 and H_2O) and metal precursors (such as trimethylaluminum-TMA, titanium tetrachloride-$TiCl_4$) on graphene surfaces. The characterization scheme used is packaged back-gated graphene-FETs which can detect the molecules adsorbed on the graphene surface. We will compare exfoliated graphene and chemical vapor deposited (CVD) graphene. Using such real-time electrical measurements, the observed charge scattering mechanisms and the effect on mobility and doping due to the interaction of these molecules with graphene will be presented.

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P14

Impact of oxygen on the electronic structure of InP (001)-(2x4) surface and InP (001)/HfO_2 (001) interface

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A theoretical study on the interaction of oxygen atom on InP(001)-(2x4) surface and InP(001)/HfO_2 (001) interface was performed using density functional theory method. Our result on surface oxidation shows that the replacement of In/P with oxygen induces the gap states in the bulk band gap whereas the oxygen adsorption does not induce the gap states due to saturation of surface dangling bonds. It also shows that the stability of the surface increases with the increase of oxygen content on the surface indicating a strong tendency for oxidation. Based on the surface oxidation model study, we have also examined the InP/HfO_2 modeling interface electronic structures under varying oxidization condition. This study helps to understand the origin of surface gap states upon oxidation of the surface and interfacial gap states when InP is interfaced with HfO_2. We also plan to compare with the experimental data to elucidate the microscopic mechanisms of the gap state development and possible approaches to control them.

P15

Surface functionalized TiO_2 Nanotubes and Thin Films for Biosensor Applications

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Titanium dioxide (TiO_2) is utilized in several applications such as biosensors, solar cells and photocatalysts, taking various forms as nanotubes and thin films. Particularly, it is attractive as a bio-compatible material since it is nontoxic. Fabrication of TiO_2 nanotubes and thin films have been formed with using atomic layer deposition (ALD), and in the case of nanotubes, an anodized aluminum oxide (AAO) nanotemplate is used as the substrate to acquire the desired tube shape [1,2].

To use the TiO_2 nanotubes and thin films as biosensors, the surfaces must be functionalized to give them the ability to selectively detect specific biomolecules. Surface modification can make TiO_2 nanotube detect specific chemicals selectively. In order to enhance their performance, we treated surface with various type of chemicals having diverse terminal group such as organosilane and carboxylic acid. Presently, we have evaluated TiO_2 nanotube and thin film biosensors functionalized with biotin in order to measure their selectivity for detecting streptavidin. The sensors have successfully detected Streptavidin. However, only improving selectivity is insufficient to produce high performance sensors because it should work under low concentration. To improve detection limit, TiO_2 should be more sensible according to environmental changes. Regulating dimension of the nanotubes make it find optimized value for each specific chemical and biological materials.

In this presentation, we will elaborate the fabrication process for both types of biosensors, demonstrate their performance as a function of device dimensions, and suggest possible sensing and conduction mechanisms.

This research was supported by a grant(code #: 2011K000211) from the 'Center for Nanostructured Materials Technology' under '21st Century Frontier R&D Programs' of the Ministry of Education, Science and Technology, Korea.

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P16

Switching Kinetic and Fatigue Property of Poly(vinylidene fluoride-trifluoroethylene) based ferroelectric capacitor

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The material properties of Poly(vinylidene fluoride-trifluoroethylene) copolymer [P(VDF-TrFE)] thin film have been studied and the process for metal-ferroelectric-metal (MFM) capacitor based on P(VDF-TrFE) have been developed and optimized. For 100 nm P(VDF-TrFE) MFM capacitor, the ferroelectric switching polarization reversal behavior for devices biased above the coercive field was mathematically modeled using the nucleation-limited-switching model in time domain. The exponential relationship between switching time and applied electric field indicates nucleation dominated switching kinetics [1]. For fatigue properties, polarization switching kinetic was studied before and after the electric stress. It was found that the increase of the polarization switching activation field and the creation of un-switchable polarization are the two major electric effects during fatigue. The increase rate of the activation field is a function of applied electric field and becomes faster as the electric field increases. For the un-switchable polarization, it keeps at around 10% of the initial polarization at all the characterization electric fields and frequencies [2]. It is demonstrated that for certain working conditions, our optimized ferroelectric thin film capacitor shows stable switching polarization and acceptable fatigue degradation compatible with flexible electronics applications. Moreover, integration of this memory element into 1T1C memory bit and 2T2C based FRAM array using inorganic thin film transistor are also demonstrated.

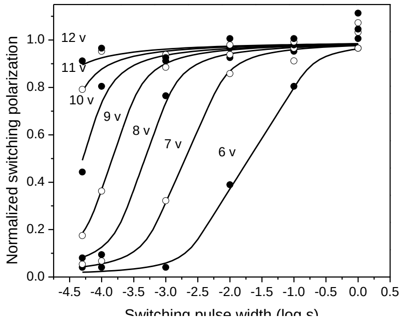

Figure 1 Experimental data of normalized switching polarization (dots) and fit data of Nucleation-limitation-switching (NLS) model as a function applied pulse width in positive region.

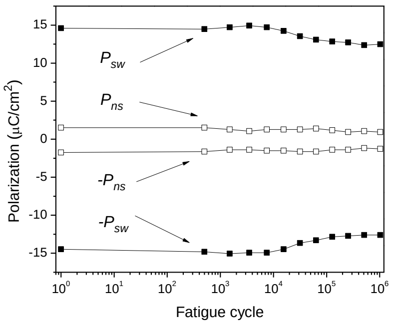

Figure 2 The degradation of switching and nonswitching polarizations in positive and negative directions as a function of stress cycle.

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P17

Characterization of CdS thin films grown by Pulsed Laser Deposition

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In this work we report Cadmium Sulphide (CdS) thin films grown by Pulsed Laser Deposition (PLD) at room temperature. This technique is used to deposit the CdS films using a set up shown in Figure 1. CdS is deposited using different pressures of argon and controlling the thickness of the films by modulating the number of laser pulses. Material characterization is carried out using primarily XRD, SEM and XPS.

The resistivity of the films was measured using a Circular Transfer Length Method (CTLM) in patterned CdS layers. Transistors were also fabricated by shadow mask and lift-off to further study the CdS films. We demonstrate that the deposition pressure is critical to control the resistivity of the resulting CdS films. A change in more than 10^6 orders of magnitude in the resistivity of the films is observed for pressure ranging from 1 to 100 mTorr, shown in Figure 2. Also, the optimum pressure for CdS films for transistor fabrication is identified and the resulting characteristics of the transistors are reported. The huge change in the resistivity of the films is related to internal stress resulting from a nano crystalline to crystalline phase in the resulting CdS films.

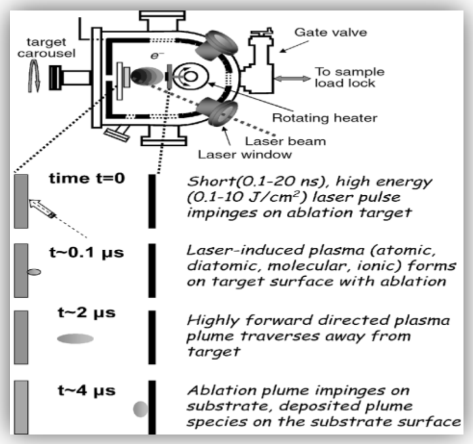

Figure 1. Schematic of the PLD process.

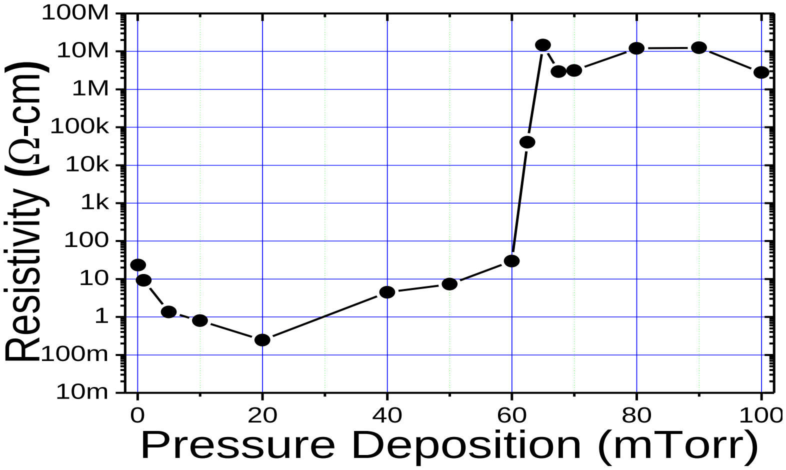

Figure 2. Resistivity of CdS thin films.

P18

Optimizing the transfer process for CVD-grown graphene

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Graphene grown by chemical vapor deposition on copper substrates provides a promising route to synthesize the large area single layer graphene that will be required if it is to be implement into production scale devices [1]. Transferring the CVD graphene to an insulating substrate is required in order to isolate the device and many groups [2,3] use similar methods to achieve this. One of the most successful variations involves coating the graphene with PMMA before etching away the original growth substrate. The graphene is then placed on the desired substrate using the PMMA as a 'handle', which is then subsequently removed. To date, a limitation of CVD graphene has been the difficulty in achieving comparable mobilities to exfoliated graphene on a given substrate [4].

While the choice of substrate is known to limit the achievable mobilities, previous work has shown that the minimization of moisture and PMMA residue is also important in maximizing the graphene mobility [3,4]. In this work, variations on the previously reported transfer process and a range of post transfer cleans are studied utilizing x-ray photoelectron spectroscopy, Raman spectroscopy, atomic force microscopy and back-gate mobility measurements with a view to further optimizing the transfer process and improving device mobilities.

Figure 1 (a) shows 3 overlapping spectra acquired from transferred graphene on SiO_2. The similarity of the spectra gives evidence to the repeatability of the transfer process. However Figure 1 (b) shows the variation in the C 1*s* spectra for different, post transfer, cleaning methods and suggests that detailed studies to indentify and understand the optimum transfer and cleaning methods is required.

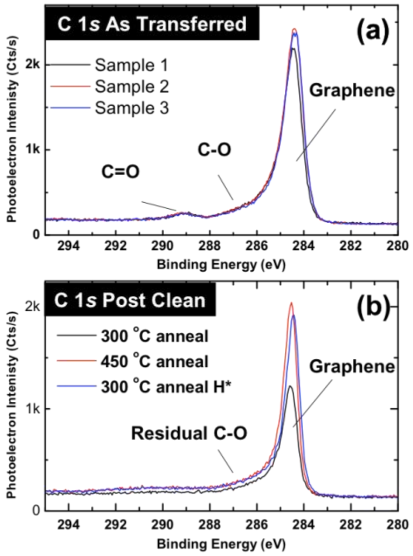

Figure 1 C 1s core-level spectra for (a) as transferred graphene onto SiO_2 and (b) post UHV cleaning (i.e. 300 °C anneal, 450 °C anneal, 300 °C anneal in Atomic hydrogen)

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P19

Modeling and SPICE Simulation of Hybrid CMOS-TFTs for Flexible Electronics

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In this work we demonstrate an accurate method to simulate the behavior of hybrid complementary metal-oxide-semiconductor thin film transistors (CMOS-TFTs) fabricated with cadmium sulfide (CdS) and pentacene as n-type and p-type active layers, respectively [1]. Both devices were fabricated using a bottom gate configuration and top source-drain (SD) contacts defined using a full photolithographic process. In particular, we describe the effect of semiconductor defects using the effective medium approach, which considers a localized charge distribution in the bandgap of the semiconductor [2]. Then, we use the unified model and parameter extraction method (UMEM) [3] to obtain the parameters of both types of transistors and introduce them into HSPICE to first simulate isolated p- and n-type TFTs and then predict the CMOS inverter behavior. Finally, we compare the experimental voltage transfer curve of the inverter as well as its gain with the HSPICE simulation, see Fig. 1. This procedure is well suitable to predict and design complex circuits based on a novel technology totally compatible with flexible electronics.

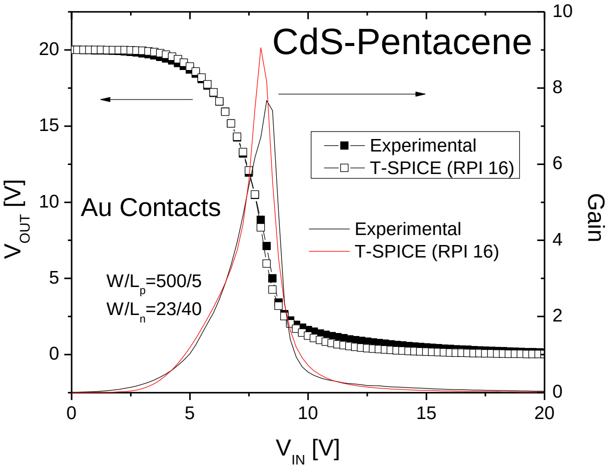

Fig.1. Experimental and simulated data of a hybrid CMOS inverter using CdS as n-type and pentacene as p-type TFT.

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P20

Graphene on a Ferromagnet: epitaxial growth and spin transparency of monolayer graphene on Cobalt on W(110)

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We have established a growth recipe for single layer graphene in a thin film of Cobalt (20 atomic layers) on W(110) through chemical vapor deposition (CVD) with ethylene (C_2H_4) at elevated temperatures of 600°C – 800°C and observed magnetic properties of graphene on Cobalt.

During the growth process four phases are involved: (i) the clean Cobalt film, (ii) a carbidic phase which exhibits a (4x4) superstructure (iii) single layer graphene and (iv) a halo like area which we interpret as a carbon depletion zone around the growth front of graphene flakes.

This behavior suggests that the mechanisms for CVD growth of single layer graphene on Cobalt are similar the recently published corresponding growth process of graphene on Nickel [1]

The domain pattern present before the growth remains largely unchanged by the graphene layer. However the observed energy dependence of the magnetic asymmetry changes dramatically after coverage with graphene.

We suggest, that this behavior is rooted in the combination of the band structure of graphene and the electronic states which contribute to the spin asymmetry in Cobalt.

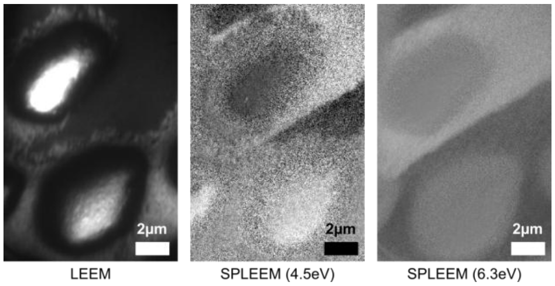

Figure 1: **(a)** LEEM image of two graphene flakes, each surrounded by the halo and a patch presumably carbide covered cobalt. **(b)** SPLEEM image (4.5eV) of the same area as in (a) and (c). The magnetic asymmetry of the underlying Co-film shows, that the flakes reside on two different magnetic domains. The asymmetry measured for the graphene flakes is opposite of the asymmetry of the underlying film. **(c)** SPLEEM image (6.4 eV) of the same area as in (a) and (b). Magnetic contrast is blocked on areas which are covered by graphene.

P21

Wet chemical approach for amino functionalization of Si(111) surfaces

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A well-defined and stable Si-N interface free from oxygen and carbon has a high impact both fundamentally and from an applied standpoint with such a surface applying in a variety of fields, ranging from medical to semiconductors. The Si-N bond is of interest due to not being susceptible to oxidation, while it provides a versatile functionality for chemical modification. Although the creation of a well defined and stable interface for the Si-N bonds has remained elusive, chlorosilanes have been shown to easily react with gas-phase or liquid ammonia and also primary and secondary amines to achieve the wanted silicon nitride bond.

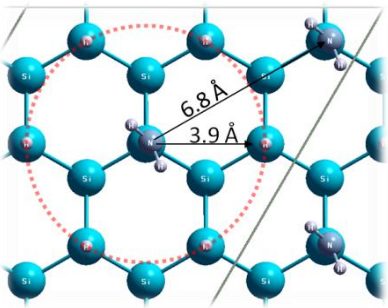

Figure 2: Top view of the proposed structure of the 1/3 amino-terminated Si(111) surface.

If instead a fluorosilane was used, preliminary calculations indicate that the kinetic barrier for the reaction of NH_3 reaction with Si-F surfaces is only slightly higher than for Si-Cl surfaces, suggesting that reactions could be induced at moderate temperatures (<70°C). Using a 1/3 ML Si-F and 2/3 ML Si-H nanopatterned model surface with a tailorable distance between Si-F groups (from 6.8 Å for 1/3ML to 3.9 Å at higher coverages), the adsorption mechanism can be investigated in detail (and evaluated by DFT calculations) and the role of NH_x-NH_x interactions explored. The ability to functionalize H-terminated Si surfaces with NH_2 groups will be crucial for a number of applications, such as biomedical (bio-sensors), solid diffusion barrier films, single electron devices, MOSFETs and MEMS while a fundamental understanding of the reactions on sparsely covered surfaces will provide the essential knowledge for progress in this field.

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P22

Model conversion reaction: Li reactivity on iron oxifluorides

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Transition metal (TM-) fluorides have gained interest as choice materials for conversion reaction-based batteries. Owing to their large band gaps and their ability to store up to three electrons per formula unit, batteries using these materials operate at high voltages and enable high energy densities.[1] However the large band gap inhibits charge conduction and thus impedes efficient charging and discharging cycles. Two paths have been taken to overcome this limitation: 1) The use of nanoparticles embedded into a conducting carbon matrix improves both ionic and electronic conduction; and 2) The use of metal oxifluorides, which are characterized by a slightly reduced energy gap that facilitates electronic conduction. It is the latter point that that is central to this study as, curiously, relatively little is known about the electronic structure of metal oxifluorides and their interaction with Li– a key aspect of a storage cell's electrochemistry.

In this work, we examine the occupied and unoccupied electronic structure of model TM fluorides and oxifluorides systems using X-ray and UV photoemission spectroscopies as well as inverse photoemission spectroscopy. Of all the metal fluorides, iron based compounds are the most promising class of fluorides with regard to maximizing energy density.[2] In order to explore initiation of the conversion process, atomic Li has been evaporated in-situ on ultra-thin FeF_xO_y films. The local chemistry upon Li deposition is interpreted from the experimental electronic structure. The morphology and phase alterations are explored using transmission electron microscopy. These results are compared to conversion reaction in electrochemical cells.

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P23

Carbon Nanotube Electrodes for Neural Interfaces

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A major challenge in the field of neuroscience is the ability to measure nervous system communications during chronic (>1 year) studies[1]. Recording fidelity is primarily lost because of the mechanical mismatch between the interface and soft nervous system tissue that leads to scar tissue encapsulation of the electrode. Furthermore, implant size limitations restrict the electrochemical properties necessary for enhanced selectivity of single unit activity[2].

Here, the development of a fully organic, chronic, central nervous system recording interface will be discussed. Cortical probes are fabricated using full photolithography on a thermoresponsive polymer substrate that is stiff enough for insertion (1 GPa) but then soften *in vivo* to approach the modulus of cortical tissue (10-100kPa). Electrodes are defined by single-wall carbon nanotubes (SWCNTs) made by chemical vapor deposition (CVD)[3] and are incorporated by a novel transfer-by-polymerization process. A comparison of the electrochemical properties of SWCNT electrodes, standard gold electrodes, and metal microwires will be made.

SWCNT electrodes on a thermoresponsive polymer substrate demonstrate that a softening substrate, lower impedance, and increased charge injection capacity will lead to an enhanced brain-machine interface.

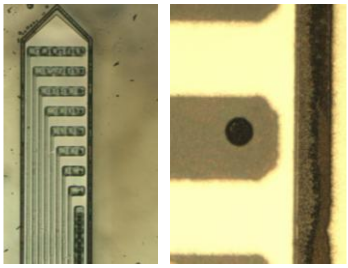

Fig. 1. Optical microscope images of a neural interface made entirely of CNT electrode conduction lines that show (a) fully lithographically defined 9-electrode array (200µm scale bar) and (b) a 15 µm recording site (50µm scale bar).

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P24

Stability and Hydrolyzation of Metal Organic Frameworks with Paddle-Wheel SBUs upon Hydration

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Instability of most prototypical metal organic frameworks (MOFs) in the presence of moisture is always a limitation for industrial scale development. In this work, we examine the dissociation mechanism of microporous paddle wheel frameworks (see Figure 1)M(bdc)(ted)$_{0.5}$ [M=Cu, Zn, Ni, Co; bdc= 1,4-benzenedicarboxylic acid; ted= triethylenediamine] in controlled humidity environments. Combined *in-situ* IR spectroscopy, Raman, X-ray diffraction measurements and first principles theoretical van der Waals density functional (vdW-DF) calculations show that the stability and modification of isostructual M(bdc)(ted)$_{0.5}$ compounds upon exposure to water vapor critically depend on the central metal ion. A hydrolysis reaction of water molecules with Cu-O-C is observed in the case of Cu(bdc)(ted)$_{0.5}$. Displacement reactions of ted linkers by water molecules are identified with Zn(bdc)(ted)$_{0.5}$ and Co(bdc)(ted)$_{0.5}$. In contrast, Ni(bdc)(ted)$_{0.5}$ is less susceptible to reaction with water vapors than the other three compounds. In addition, the condensation of water vapors into the framework is necessary to initiate the dissociation reaction. These findings provide the necessary information for determining operation conditions of this class of MOFs with paddle wheel secondary building units and guidance for developing more robust units.

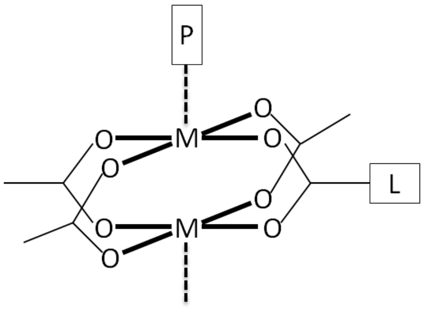

Fig. 1. Schematic illustration of coordination geometry of paddle wheel building units: M= Metal ion, L=Bicarboxylate linker and P= N-containing bidentate pillar linker

P25

Characterization of Few Layer Graphene films Grown on Cu-Ni and SiC Substrates

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C. Dimitrakopoulos[3], A. Grill[3], C. Y. Sung[3], S. Chen[4], A. Munson[4], Y. Hao[4],
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The electronic structure of graphene depends on the number of graphene layers and the stacking sequence between the layers. Therefore, it is important to have a non-destructive technique for analyzing the overlayer coverage of graphene directly on the growth substrate. We have developed a technique using angle-resolved XPS to determine the average graphene thickness directly on metal foil substrates and SiC substrates. Since monolayer graphene films can be grown on Cu substrates, these samples are used as a standard reference for a monolayer of graphene. HOPG is used as a standard reference for bulk graphite. The electron mean free path of the C-1s photoelectron can be determined by analyzing the areas under the C-1s peaks of monolayer graphene/Cu and bulk graphite. With the measured electron mean free path, the graphene coverage of a film of arbitrary thickness can be determined by analyzing the area under the C-1s of that sample. Analysis of graphene coverages for graphene films grown on Cu-Ni substrates and of the thickness of both the graphene overlayer and intermediate buffer layer on SiC will be presented. In addition, Raman spectroscopy measurements of the graphene films were made and correlate well with the coverages determined by angle-resolved XPS. This research was supported in part by the National Science Foundation (grant no. 1006350/1006411).

P 26

Chemical and Electrical Passivation of Silicon Surfaces through Hydrosilylation and Chlorination Reactions

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Hydrogen-passivated Si(111) surfaces are produced through two different preparation methods: modified RCA and HF treatment. The two types of surfaces have been examined by infrared spectroscopy (IR) X-ray photoelectron spectroscopy (XPS) and charge-carrier lifetime measurements, and display different chemical and electrical properties. The HF treatment yields long charge-carrier lifetime and low surface recombination velocity, but atomically rough surface. The modified RCA method produced chemically well-defined mono-hydride silicon surface with relatively poor electrical properties. The two types of surfaces produced were further subjected to modification with chlorine (PCl_5) and alkene monolayers (C11 and C18). The chemical and electrical properties, surface structure, and chemical reactivity of the surfaces have been investigated by X-ray photoelectron spectroscopy, IR, and atomic force microscopy. The procedures for surface preparations and modifications will be discussed.

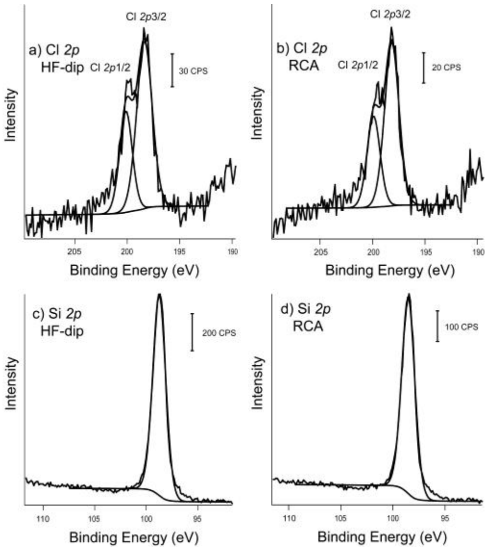

Figure 1. XPS investigation of Cl-Si(111) surfaces produced by HF-dip ((a) Cl *2p* edge and (c) Si *2p* edge) and RCA ((b) Cl *2p* edge and (d) Si *2p* edge) surface preparation procedures.

P27

Environment controlled tethering by aggregation and growth of phosphonic acid monolayer on silicon oxide

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Phosphonic acid monolayers are being considered as versatile surface modification agents due to their unique ability to attach to surfaces in different configurations, including mono-, bi- or even tridentate arrangements. Tethering by aggregation and growth (T-BAG) of octadecylphosphonic acid (ODPA) on silicon oxide surfaces has proven to be a robust method to establish a strong chemical bond. However, it requires a long processing time (> 48h) that has present a substantial drawback for industrial applications. We demonstrate here that the humidity level during processing is the most important parameter controlling the reaction. Using in situ infrared absorption spectroscopy, we first show that the initially physisorbed layer obtained upon immersion in ODPA is composed of well-ordered bilayers and only reacts with the SiO_2 surface at 140^{o}C. Importantly, we show that the presence of water at the interface (determined by the humidity level) greatly influences the reaction time and completion. In humid environments (relative humidity, RH > 40%), there is no reaction, while in dry environments (RH < 16%) the reaction is essentially instantaneous at 140^{o}C. Ab initio calculations and modeling confirm that the degree of chemical reaction with the surface OH groups depends on the chemical potential (i.e. concentration) of interfacial water molecules. These findings provide a workable modification of the traditional T-BAG method consistent with many industrial applications.

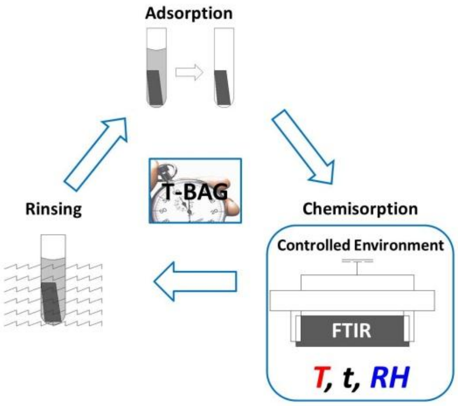

Fig. 1. Schematic diagram of the modified T-BAG method.

P28

TERNARY THIOL-ENE-ACRYLATE SUBSTRATES FOR SOFTENING NEURAL INTERFACES

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Silicon-based neural interfaces have been shown to have poor stability during chronic implantation[1]. This failure general failure of electronic devices, usually within a year of implantation, has been largely attributed to the extreme mechanical mismatch between the silicon substrate and neural tissue. Advances in the field of flexible electronics, using polymers as substrates, have been readily incorporated in the design of neural interfaces. In this work a dimensionally-stable, smart polymer capable of softening in response to physiological conditions, despite low water uptake, is developed. Substrates are designed to remain in the high modulus, glassy during implantation and soften after implantation. Control of the glass transition temperature and modulus in physiological conditions is achieved through varying diacrylate content from 0 – 31 mol%. The shear modulus under simulated physiological conditions increases with diacrylate content from 6.5 to 80 MPa. Intracortical probes (Figure 1) and other types of implantable microelectrode arrays are fabricated, implanted and used in acute recordings. These substrates are the first example of substrates that soften considerably in physiological conditions, but maintain compatibility with standard photolithographic processes. Devices are fabricated with a novel process that allows for control of the metal-polymer interface. The physiological response of these polymers, combined with excellent tolerance to photolithographic processes, makes this a promising system of substrates for neural interfaces that decrease the mechanical mismatch at the biotic-abiotic interface while offering increasingly advanced device capability.

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P29

Temperature Dependence of DNA Charge Transport

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Charge transport (CT) through DNA has been extensively studied, and yet the mechanism of this process is still not yet fully understood. DNA CT has been utilized in sensing proteins and DNA fragments, and it has been postulated that it may assist DNA damage prevention and repair. Besides the benefits of understanding charge transport through this fundamental molecule, further understanding of this process will elucidate the biological implications of DNA CT and advance sensing technology. Therefore, we have investigated the temperature dependence of DNA CT by measuring the electrochemistry of DNA monolayers modified with a redox-active probe.

By using multiplexed electrodes on silicon chips, we compare square wave voltammetry of distinct DNA sequences under identical experimental conditions. Accordingly, we compare well matched DNA duplexes to those containing a single base pair mismatch, which has been shown to attenuate CT. Furthermore, we couple the redox probe at distinct positions within the well matched DNA duplex in order to investigate distance dependent kinetics. Using a model put forth by O'Dea and Osteryoung and applying a nonlinear least squares analysis we are able to determine the charge transfer rates (k), transfer coefficients (α), and the total surface concentration (Γ^*) of the DNA monolayer. The transfer rates of CT are shown to follow Arrhenius behavior, with increased activation energies for mismatches that structurally distort the duplex. These observations suggest that charge transport is thermally activated and highly dependent upon DNA conformation.

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P30

Impact of oxygen on the electronic structure of GaSb(100) surface and GaSb(100)/HfO$_2$(001) interface

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Antimony-based III-V semiconductors such as GaSb have attracted research attention in recent years for the applications in metal-oxide-semiconductor field effect transistors (MOSFETs) and heterojunction tunnel field effect transistors (H-TFETs) due to its high mobility [1]. Since both applications require integrating high dielectric constant (high-k) oxides on the semiconducting channel materials, the interface quality between these oxides and III-V compounds is crucial to the device performance. For this purpose, we investigate at the atomic level the mechanisms of GaAs(100) surface oxidation and the origin of interface states of GaSb(100)/HfO$_2$(001)interface by first principles calculations. These modeling methods have been successfully applied in the previous study of the GaAs systems [2]. Our preliminary results show that for GaSb surface oxidation, the adsorbed oxygen atom satisfies the bond saturation condition and do not introduce surface gap states. In contrast, the Sb-substituted oxygen atom could either induce gap states or do not be harmful to the GaSb surface electronic structure, depending on where it stays. GaSb/HfO$_2$ modeling interface systems are also investigated to develop a detailed understanding on the interface state formation and possible approaches to control them.

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P31

Electronic Reconfiguration of Graphite to Graphene through Vertical Displacement of the top layer

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Scanning Tunneling Microscopy (STM) measurements were taken on highly oriented pyrolytic graphite (HOPG) with the STM in constant current mode. The potential bias of the tip was varied, similar to a Scanning Tunneling Spectroscopy measurement, and the height of the tip was measured as function of the tip bias. The tip moved 35 nm during a voltage sweep of 0.1 to 5 V, indicating that the top layer of graphite had decoupled from the surface. 150 nm by 150 nm STM images were taken before, during and after the STS measurement, and large scale deformations were found on the surface (Fig 1) supporting this finding. More STM atomic resolution (6 nm by 6 nm) images were taken on HOPG and revealed a variety of charge densities on the surface, including the typical triangular structure associated with HOPG surface, the honeycomb structure typically associated with graphene, as well as hybrid structures. Density Functional Theory calculations were used to simulate STM images of a 6 layer Bernal-stacked graphite. The height of the top layer of graphite was systematically increased, and a continuous transition to graphene was observed at a vertical displacement of 0.150 nm.

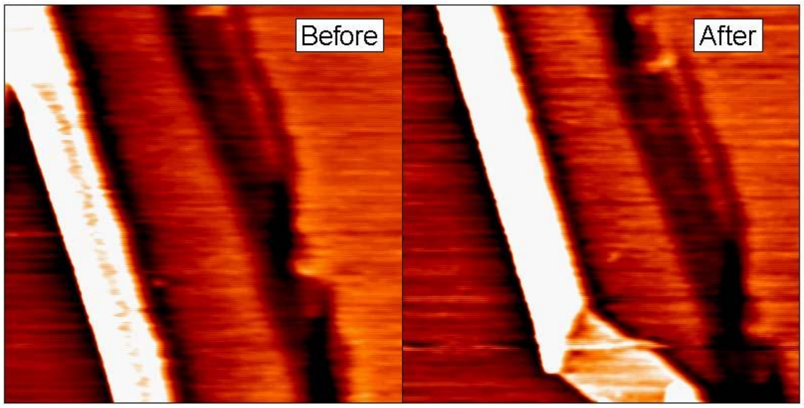

Figure: 150 nm by 150 nm Filled State STM images taken of HOPG. (Left) Image taken before doing constant-current STS measurements on the sample. STS measurements were taken along the left-hand side of the white stripe. The indentation in the trench along the right hand side of the image allows comparison between images (Right) Image taken after constant current STS measurements.

This was work was supported in part by acknowledge the financial support of the Office of Naval Research (ONR) under grant number N00014-10-1-0181 and the National Science Foundation (NSF) under grant number DMR-0855358

P32

Simulation of cluster formation at low energy ion sputtering of Cu (100) and Ag (100)

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Cluster emission processes at ion bombardment of solids attract many scientists due to their unique formation mechanisms. Recently it was shown that small clusters are predominantly emitted in the collisional phase of the sputter process (for times up to 1 ps) or due to fragmentation of large cluster while large clusters (with 10 or more atoms) are emitted well after the collision cascade is thermalized, and can be understood in terms of thermal and hydrodynamic processes [1].

In the present work the formation mechanisms of small clusters at grazing ion bombardment are studied. As numerous experimental studies show that cluster formation depends on some conditions: the energy and mass of the bombarding particles, surface structure and binding energy of substrate atoms. The idea of using grazing angle ion sputtering is to transfer the same energy to several neighbor atoms in order to eject them together. We have carried out simulation, which are based on some possible models and mechanisms of cluster formation during ion sputtering of a solid surface. An interaction between atoms is described by well-defined embedded atom model. Calculations were performed for the cases of self sputtering as well as for the mixed combinations of Cu and Ag projectile-solid system. Internal and kinetic energy distributions as well as yields of particles emitted with different sizes are calculated. An influence of the initial energy varying from 0.5 to 5 keV and grazing angle (0-30^o) of incident particles to the process of cluster formation are analyzed. On the basis of obtained results and performed analysis the nature of cluster formation during grazing ion sputtering of a solid surface is discussed.

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P33

Thermal Transport in Graphene and Graphene Oxide: An atomistic simulation study

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With the continuous miniaturization and the growing integration of electronics, heat dissipation has become a critical issue that catalyzed a wide search for high thermal conductivity materials applicable in electronic devices. Over recent years, single layer graphene has been studied for its promising application in electronics not only because of its unique electron transport properties, but also due to its superior thermal conductivity as compared to other materials. Both of these features make graphene a promising material for the future generation semiconductor device technology. Among several developed techniques for graphene growth[1, 2, 3], reduced graphene oxide (rGO) method emerged as a promising approach to produce graphene in a large scale which can be favorable for practical electronics application[3,4]. In reduced GO method, one remaining challenge is that rGO can not fully restore the electric property of pristine graphene because of the difficulty in removing the residue oxygen group without causing damage to the graphene structure [4]. Based on this fact, we expect there is a similar challenge for improving thermal conductivity of rGO, which has not been well understood, yet. In this work, we apply an atomistic simulation method to model the effect of residue oxygen group on the thermal conductivity of graphene. This simulation model was used to achieve quantitative agreement with experimental data in a recent work on the thermal conductivity of isotopically engineered graphene[5]. We expect our simulation results would be a useful reference on how to modulate thermal conductivity of rGO by increasing or decreasing the surface concentration of oxygen groups. Ideally, producing low cost rGO with reasonable high thermal conductivity would help to address the heat dissipation issue in electronics.

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P34

Chemical and electrical properties of the crystalline oxide/$In_{0.53}Ga_{0.47}As$ (100) interface

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Silicon-based metal-oxide-semiconductor-field-effect transistors (MOSFETs) are facing their fundamental scaling limits beyond the 32nm node. Therefore, new alternatives for channel and gate-insulator materials have been under intensive research. InGaAs is a proposed channel material for future generations of MOSFETs due to its superior electron mobility compared to Si. Significant efforts have been undertaken to engineer gate-insulator interfaces with InGaAs channel layers that are stable and meet industry-device criteria as the SiO_2-Si junction does.

Recently it was shown that it is possible to form a crystalline oxide on III-V surface layers by controlled oxidation of the III-V surface[1]. In this study we investigate the properties of the $In_{0.53}Ga_{0.47}As$(100)/crystalline oxide interface, which is of critical importance since the presence of interfacial states such as surface dimers or dangling bonds can impact significantly on device performance. The crystalline oxide on the InGaAs surface is formed *in situ* by removing an arsenic capping layer and exposing the sample to an oxygen environment at 420 °C (fig.1). The growth of the oxide layer is then monitored using monochromatic X-ray photoelectron spectroscopy. Al_2O_3 is subsequently deposited on the oxidized surface in order to fabricate metal-oxide semiconductor capacitors (MOSCAP) for electrical characterization. Results on the interfacial chemistry and structure of the oxide will be presented.

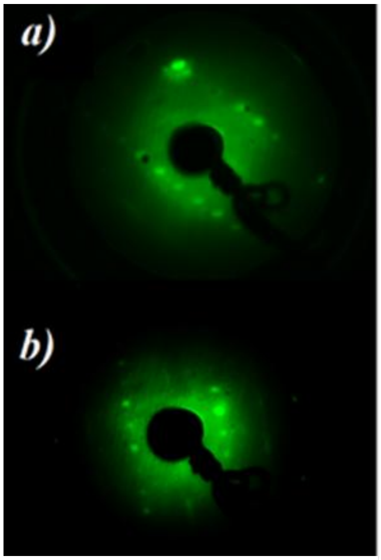

Figure 1. LEED pattern of InGaAs surface after (a) As-decapping and (b) after oxidation

The authors acknowledge useful discussions with Dr. P. Laukkanen (Univ. Turku). This work was supported by the Semiconductor Research Corporation (SRC) FCRP Materials Structures and Devices (MSD) Center, the SRC Nanoelectronics Research Initiative and National Institute of Standards & Technology through the Midwest Institute for Nanoelectronics Discovery (MIND), and the National Science Foundation (NSF) under ECCS award 0925844.

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P35

-NH- Termination on Si(111) Surface through Ammonia Treatment

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Silicon surface modification based on Si-N bonds has been investigated for over a decade; however, the obtained surfaces tend to have additional carbon or oxygen contamination. Here we present a new method to functionalize Si(111) surfaces with –NH- termination by wet chemistry methods at room temperature. The experiment scheme is shown in Figure 1: we start with a single Si(111) crystal surface covered with native oxide. After the classic RCA cleaning cycle, Si(111) surface is etched with HF/NH_4F to form a hydrogen-terminated Si(111) surface. The resulting sample is treated with PCl_5 in chlorobenzene to form Cl-terminated Si(111) according to reference [1]. Finally, the sample is treated with NH_3/THF solution in inert atmosphere to obtain the –NH- termination on Si(111) surface. In order to confirm the identity of surface products during each modification step, the chemistry was monitored by infrared spectroscopy (IR) and X-ray photoelectron spectroscopy (XPS). In addition, density functional theory (DFT) calculations were applied to predict N *1s* core level energy and evaluate the possible reaction mechanisms. The Si-NH-Si as the main species was identified by IR, XPS and time-of-flight secondary ion mass spectrometry (ToF-SIMS). The quantitative surface coverage was also calculated based on XPS results, which indicated that the chlorine coverage reached 99% on Cl-terminated Si(111) surface and all the chlorine atoms were replaced with nitrogen-containing functionality, at a ratio of two chlorine atoms per one nitrogen, corresponding to the Si-NH-Si species formed [2].

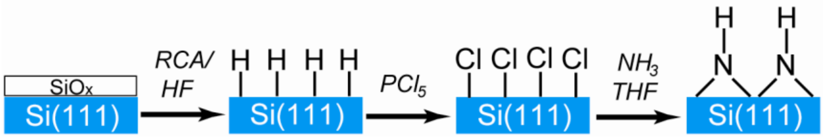

Figure 1. Scheme of the preparation steps to form a –NH-terminated Si(111) surface.

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P36

Optical Spectroscopy of Thin Films by Using Azimuthal and Radial Polarizations

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Tight focusing of an azimuthally polarized laser beam generates transverse electric field at the focal spot, while there also exists an intense longitudinal electric field for a focused radially polarized laser beam [1,2]. The use of radial and azimuthal polarizations thus allows for orientation determination of single molecules, and excitation of new optical transitions and phonon modes. We performed Raman and fluorescence spectroscopy measurements on thin film materials by using azimuthal and radial laser polarizations. The thin film samples studied include few-layer graphene and mono-layer films of organic molecules such as pentacene. These thin films have well characterized and known structures, permitting us to predict their optical behaviors. Theoretical simulation of electric field distribution at laser focal region is performed, and it can explain quantitatively the observed spectral differences among different thin film samples.

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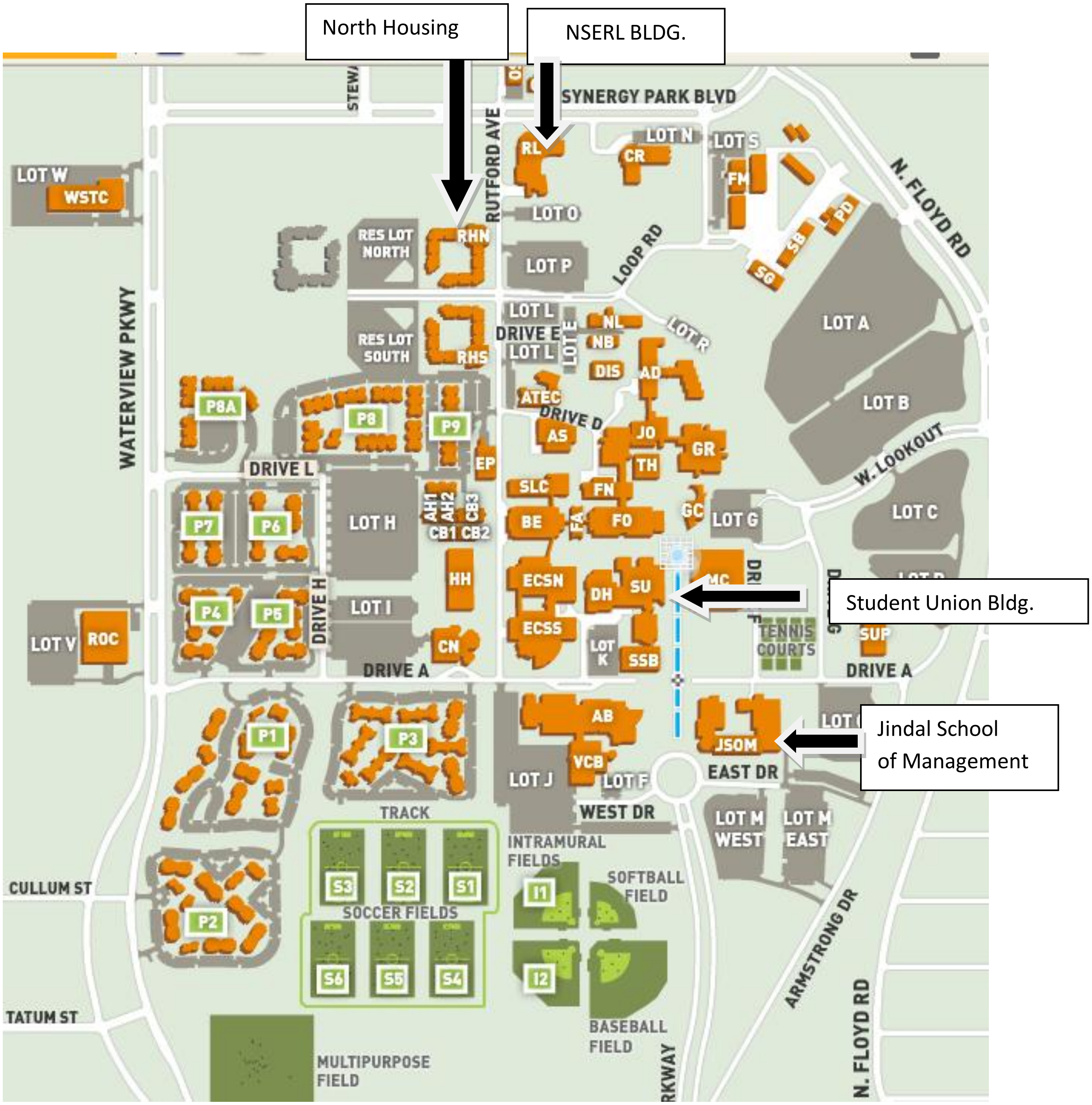
Campus Maps


North Housing

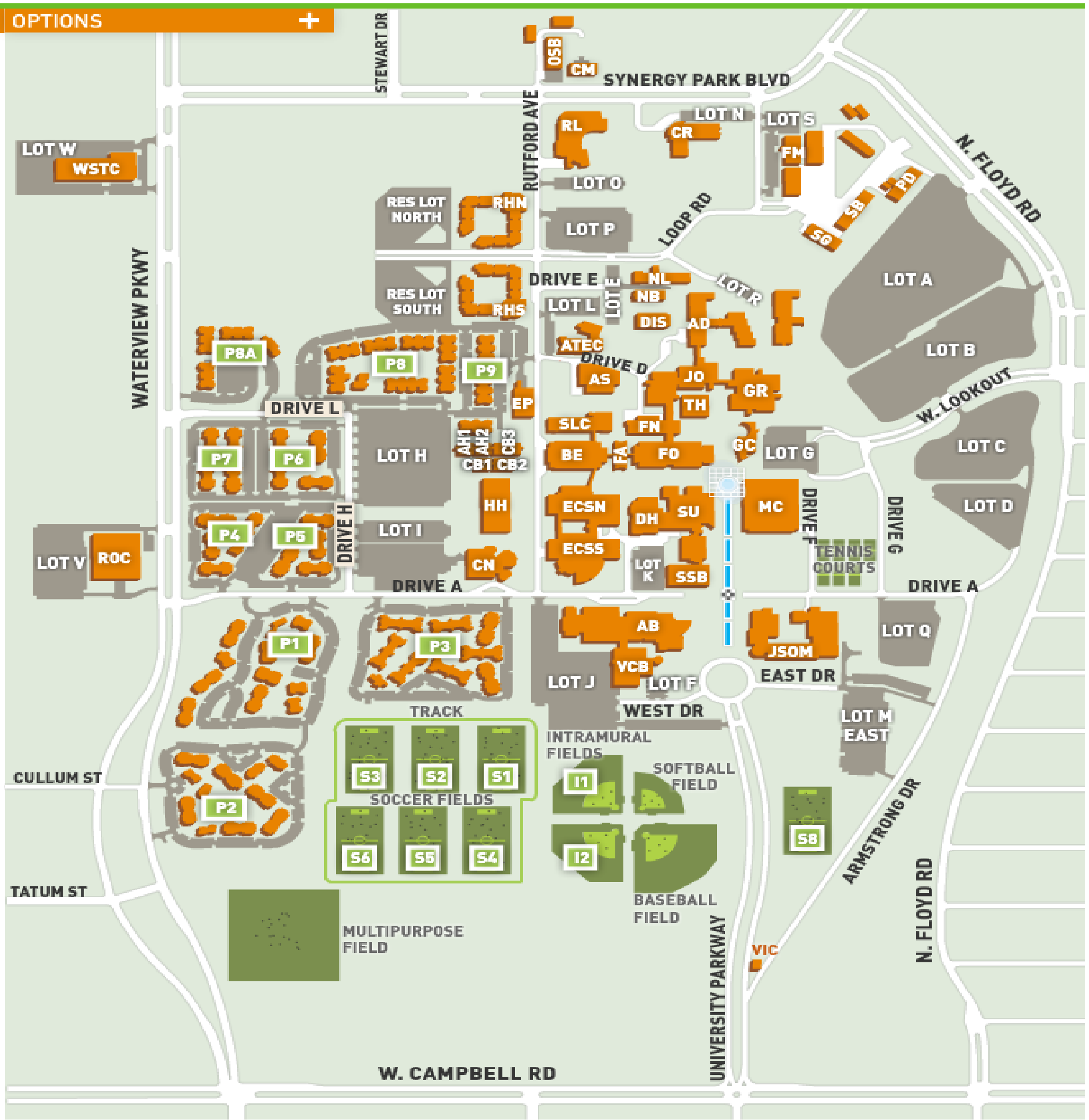
NSERL BLDG.

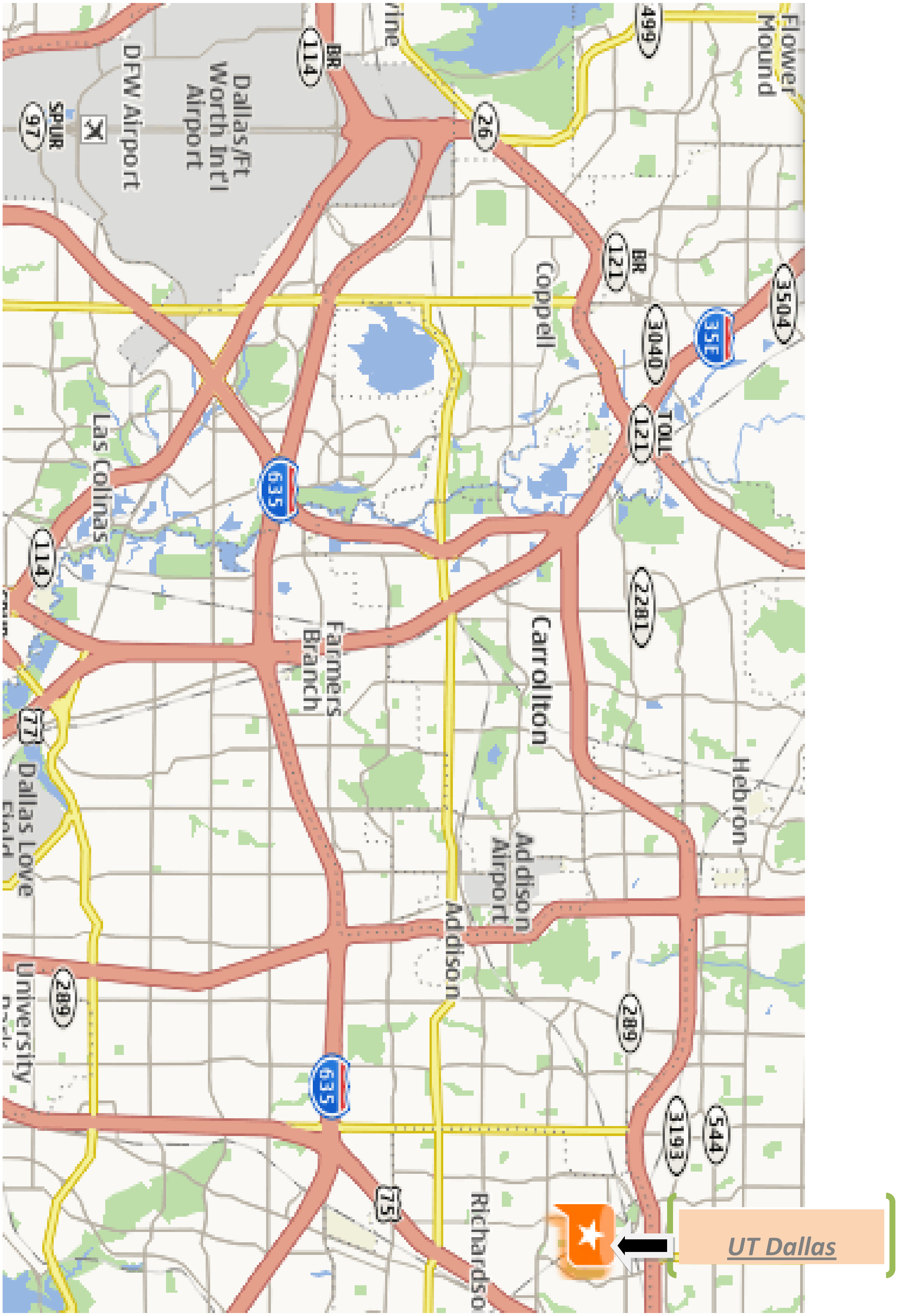
Student Union Bldg.

Jindal School of Management

BUILDINGS AND LOCATIONS

AB	Activity Center
AD	Administration
AH1	Arts and Humanities 1
AH2	Arts and Humanities 2
AS	Visual Arts Studio
ATEC	Arts and Technology Building
BE	Lloyd V. Berkner Hall
CB1	Classroom Building 1
CB2	Classroom Building 2
CB3	Classroom Building 3
CM	Construction Management
CN	Alexander Clark Center (Conference Center)
CR	Callier Center Richardson
DH	Dining Hall
DIS	Dallas International School
ECSN	North Engineering and Computer Science
ECSS	South Engineering and Computer Science
EP	Energy Plant
FA	Founders West Annex
FM	Facilities Management
FN	Founders North
FO	Founders Building
GC	Cecil and Ida Green Center
GR	Cecil H. Green Hall
HH	Karl Hoblitzelle Hall
JO	Erik Jonsson Academic Center
JSOM	Naveen Jindal School Of Management
MC	Eugene McDermott Library
NB	North Office Building
NL	North Lab
OSB	Old Service Building
PD	Police
RHN	Residence Hall North
RHS	Residence Hall South
RL	Natural Science and Engineering Research Lab
ROC	Research and Operations Center
SB	Service Building
SG	Safety and Grounds
SLC	Science Learning Center
SSB	Student Services Building
SU	Student Union
TH	Theatre
VCB	Visitor Center and University Bookstore
WSTC	Waterview Science and Technology Center

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2012 Physical Electronics Conference Program

A topical conference on the Physics and Chemistry of Surfaces and Interfaces,
72nd Annual Meeting, June 3 – 6, Department of Materials Science and Engineering, University of Texas at Dallas, Richardson, Texas

Sunday, June 3, 2012

3:00 – 5:00 PM	Dorm Check in – Residence Hall North, lobby
5:00 – 9:00 PM	Registration and Welcome Reception – NSERL lobby

Monday, June 4, 2012

7:30 - 8:30 AM	Registration and Breakfast - JSOM Atrium (Jindal School of Management)
8:30 – 8:40 AM	Opening and Welcome – Davidson Auditorium
8:40 – 10:00 AM	Oral Presentations – Davidson Auditorium
10:00 – 10:20 AM	Coffee Break - JSOM Atrium
10:20 – 12:00 PM	Oral Presentations – Davidson Auditorium
12:00 – 1:30 PM	Lunch – Galaxy Rooms (Student Union)
1:30 – 3:30 PM	Invited Lecture and Oral Presentations – Davidson Auditorium
3:30 – 3:50 PM	Afternoon Break
3:50 – 5:10 PM	Oral Presentations – Davidson Auditorium
5:10 – 6:40 PM	Poster Session – Galaxy Rooms (Student Union)
6:40 – 9:00 PM	Picnic – Student Union Mall and Reflection Pools (between Student Union and the McDermott Library

Tuesday, June 5, 2012

7:30 – 8:30 AM	Breakfast – JSOM Atrium
8:30 – 9:50 AM	Nottingham Contestant Presentations
9:50 – 10:10 AM	Morning Break – JSOM Atrium
10:10 – 11:50 AM	Nottingham Contestant Presentations
11:50 – 1:30 PM	Lunch Break – Galaxy Rooms (Student Union)
1:30 – 3:10 PM	Invited Lecture and Nottingham Contestant Presentation
3:10 – 3:30 PM	Coffee Break – JSOM Atrium
3:30 – 4:10 PM	Nottingham Contestant Presentations
4:10 – 6:30 PM	Poster Sessions – Galaxy Rooms (Student Union)
6:30 – 9:00 PM	Banquet – Galaxy Rooms (Student Union)

Wednesday, June 6, 2012

7:30 – 8:30 AM	Breakfast – JSOM Atrium
8:30 – 9:50 AM	Oral Presentations – Davidson Auditorium
9:50 – 10:10 AM	Morning Break – JSOM Atrium
10:10 – 11:30 AM	Oral Presentations
11:30 – 1:00 PM	Box Lunch – JSOM Atrium
1:00 – 4:00 PM	Tours of Local Industries (optional)
Thursday	Meeting of the UT Dallas AVS Texas Chapter (optional)