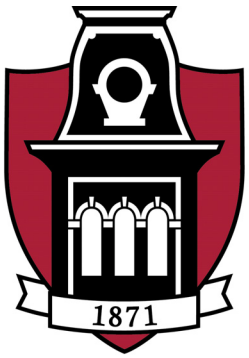

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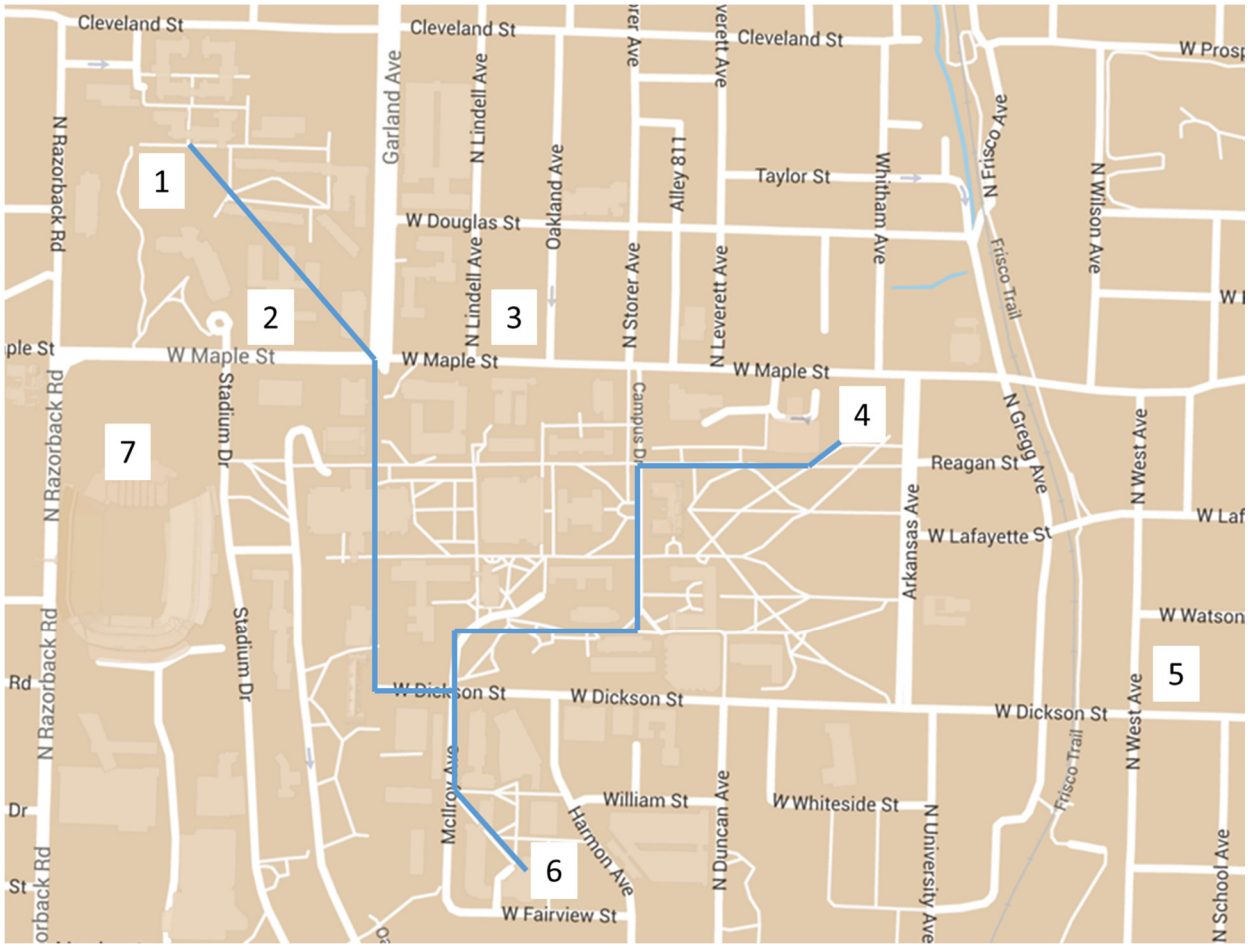
76th Physical Electronics Conference

June 20-23, 2016

Abstract Booklet

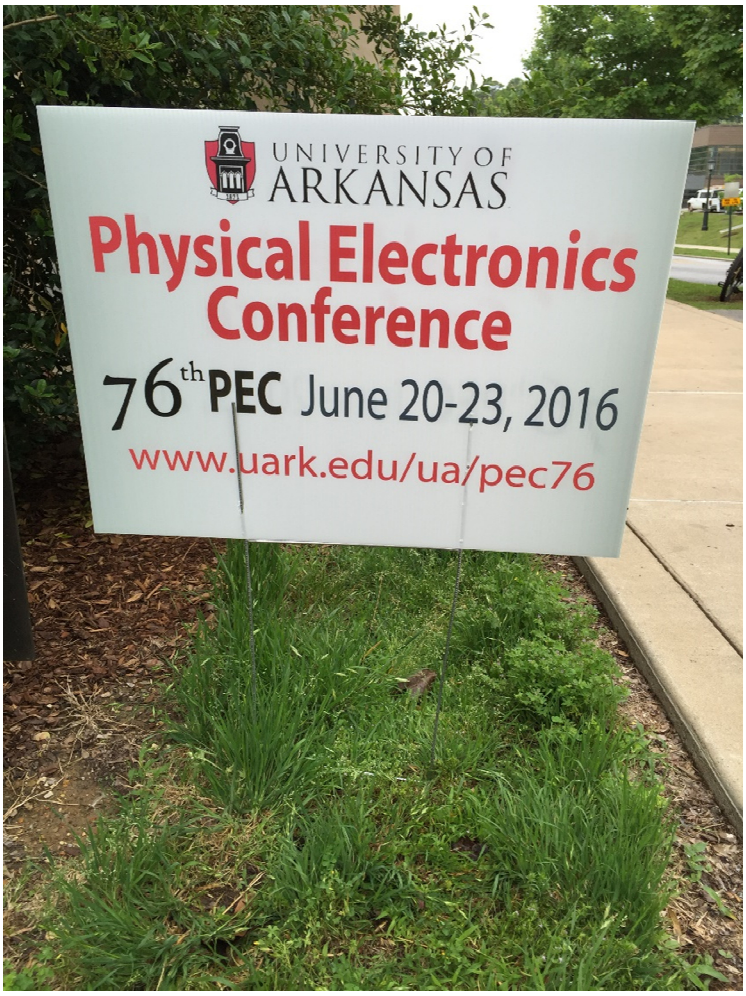
http://www.uark.edu/ua/pec76/

Campus Map



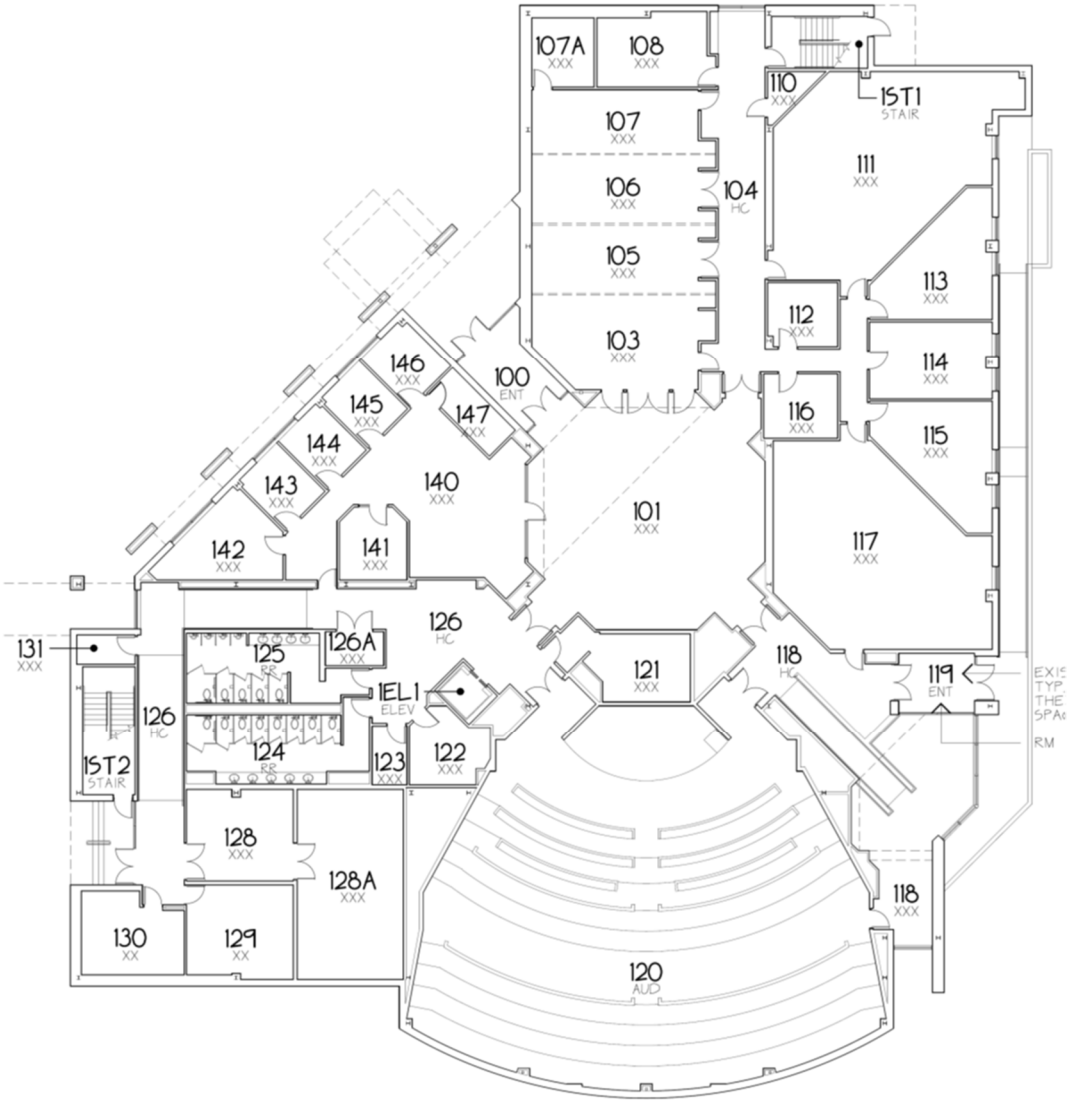
(1) Maple Hill Dorm
(2) Hawkins Family Terrace
(3) University House
(4) Inn at Carnall Hall
(5) Hog Haus Brewing Co.
(6) Reynolds Center
(7) Raymond Miller Hall of Champions

PEC Campus Signs



Look for these signs marking the various venues and pathways.

Reynold Center Floorplan



Room 103-107: Breakfast and Lunch

Room 120: Oral Presentations

Room 101: Coffee Breaks

Room 111: Poster Session

Venue Photos

Maple Hill Dorms

Inn at Carnall Hall

Venue Photos

University House

Reynolds Center

Venue Photos

Hawkins Family Terrace

Hog Haus

Venue Photos

Raymond Miller Banquet

(lower right entrance)

Raymond Miller Banquet

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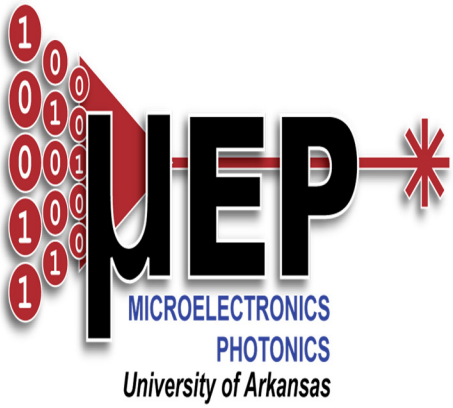
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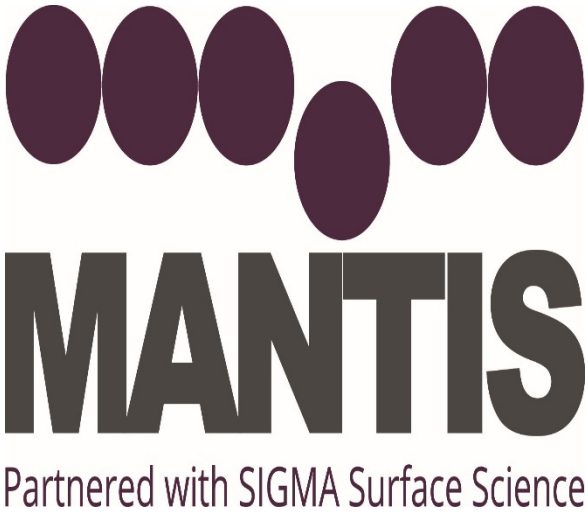
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PEC

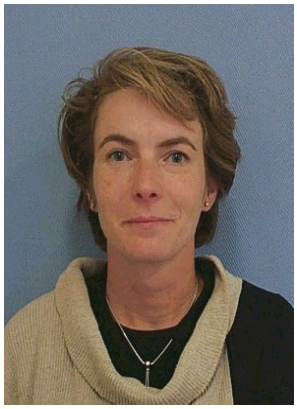
The annual Physical Electronics Conference provides a forum for the dissemination and discussion of new research results in the physics and chemistry of surfaces and interfaces. It includes the prestigious Nottingham Prize Competition for best presentation based on doctoral research.

In addition to three 40-minute invited talks, the conference will include 20-minute oral presentations in a single-session format with lively discussions. The conference's three-day format limits the total number of oral contributions to about 50, and additional contributions are included as poster presentations. With the exception of Nottingham contestants, a one-page abstract is the sole written submission required of contributors.

Invited Speakers

Prof. Jochen Mannhart

Director
Max Planck Institute for Solid State Research, Stuttgart



Prof. Agnès Barthélémy

Senior Member
Institut Universitaire of France
CNRS/Thales, Paris-Sud University

Jonathan W. Thibado

PMCI Manager
Principal Engineer
Intel Corporation

Jonathan Thibado is a Principal Engineer at Intel and leads the mechanical development of data centers (High Performance Computers, Servers, Enterprise, and Cloud). He has more than 21 years of experience with Intel's Portland Technology Development (PTD) group designing processes and manufacturing aspects of the silicon central processor, from the first Pentium to the modern Core. Jon is currently leading teams in developing mechanical components for server systems to be released in 2020 and beyond. In addition, he is leading efforts to revolutionize the industry's approach in the designs and methods for semiconductor packaging and systems.

About PEC

The Physical Electronics Conference has been held on university campuses and at research labs around North America for 75 years. The University of Arkansas has been selected to host the 76th annual Physical Electronics Conference (PEC). This topical conference provides a yearly forum for the dissemination and discussion of novel and fundamental theoretical and experimental research in the physics, chemistry, biology, and engineering of surfaces and interfaces. Presentations of PhD thesis research, made by young contestants for the prestigious Nottingham prize ($1,500), are highlighted. Representative topics include electronic, chemical, magnetic, and structural properties of surfaces and interfaces; energetics, kinetics, and dynamics of physical, chemical, and biological transformations; electron correlation at surfaces and interfaces; interactions of biological materials; mechanisms of film growth, interface evolution, and reduced dimensionality; and processes of energy, electron, ion, and molecular transfer at surfaces and interfaces.

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1966 Massachusetts Institute of Technology

1967 Massachusetts Institute of Technology

1968 University of Minnesota

1969 Yale University

1970 University of Wisconsin - Milwaukee

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1976 University of Wisconsin - Madison

1977 Stanford University

1978 Oak Ridge National Laboratory

1979 University of Maryland

1980 Cornell University

1981 Montana State University

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1983 Sandia National Laboratories

1984 Princeton University

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1986 University of Texas - Austin

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1988 Brookhaven National Laboratory

1989 University of Washington

1990 National Institute of Standards

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1993 Rensselaer Polytechnic Institute

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2005 University of Wisconsion - Madison

2006 Princeton University

2007 University of Illinois at Urbana-Champaign

2008 University of California - Riverside

2009 Rutgers University-New Brunswick

2010 University of Wisconsin - Milkwaukee

2011 University at Albany

2012 University of Texas - Dallas

2013 North Carolina State University

2014 University of Wisconson - La Crosse

2015 Rutgers University-New Brunswick

The 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 $1,500, is awarded to the best student paper 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. In addition, you and your advisor's names are added to the Nottingham Wikipedia website.

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		
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 Inst. 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)	T. Michely
2010	Heather Tierney	Tufts University	Charles H. Sykes
2011	Tanza Lewis	University of California - Irvine	J. Hemminger & B. Winter
2012	Daniel Schwarz	University of Twente	B. Poelsema
2013	Benjamin A. Gray	University of Arkansas - Fayetteville	J. Chakhalian
2014	Donna A. Kunkel	University of Nebraska - Lincoln	A. Enders
2015	Christoph Große	Max Planck Institute for Solid State Research	K. Kern
	Amanda Larson	University of New Hampshire	K. Pohl

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2016 Physical Electronics Conference Program

All oral presentations occur in the Reynolds Center Auditorium (RCED 120) located in the Donald W. Reynolds Center for Enterprise Development building. Breaks, vendors, and registration will be in the Reynolds Center atrium (RCED 101), just outside the auditorium. Posters will be displayed in room RCED 111, down the hall. Breakfast and lunch will be served in rooms RCED 103-107, adjacent to the atrium.

Monday, June 20, 2016

4:00 p.m. – 6:00 p.m.	Registration – Maple Hill Dorm (1201 Cleveland Street)
6:00 p.m. – 8:00 p.m.	Welcome Reception – University House Registration – University House

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Tuesday, June 21, 2016

7:00 a.m. – 8:00 a.m.	Breakfast – Reynolds Center (RCED 103-107) Registration (all day) – Reynolds Center (RCED atrium) Setup Posters (RCED 111)
8:00 a.m. – 8:20 a.m.	Opening Remarks (RCED 120) Prof. Jim Rankin, Vice Provost for Research & Development Prof. Julio Gea-Banacloche, Chair of Physics Department Prof. Paul Thibado, Local PEC Chair
Session 1	Moderator: Prof. Pat Thiel, Iowa State University

8:20 a.m. – 8:40 a.m.

Density Functional Theory Study of Chemical Functionalization of Two-dimensional Materials

Tong Mou [1], Bin Wang [1]

[1]School of Chemical, Biological and Materials Engineering, University of Oklahoma, Norman, OK

8:40 a.m. – 9:00 a.m.

SAD-GLAD Pt-Ni @Ni nanorods as Highly Active Oxygen Reduction Reaction Electrocatalysts

Mahbuba Begum[1], Nancy N. Kariuki[2], Mehmet F. Cansizoglu[1], Mesut Yurukcu[1], Fatma M. Yurtsever[1], Tansel Karabacak[1], and Deborah J. Myers[2]

[1]Department of Physics and Astronomy, University of Arkansas at Little Rock, Little Rock AR 72204, USA

[2]Chemical Sciences and Engineering Division, Argonne National Laboratory, Argonne, IL 60439-4837, USA

9:00 a.m. – 9:20 a.m.

Spatially Resolved Scanning Tunneling Spectroscopy of Single Layer Steps on Si(100) Surfaces: Experiment and Simulation

X.Wang[1,2], P. Namboodiri[2], K.Li[2], X.Deng[2], and R.Silver[2]

[1]Chemical Physics Program, University of Maryland, College Park, MD, 20742, USA

[2]Engineering Physics Division, National Institute of Standard and Technology, Gaithersburg, MD

9:20 a.m. – 9:40 a.m.

Interrogating the superconductor $Ca_{10}(Pt_4As_8)(Fe_{2-x}Pt_xAs_2)_5$ Layer-by-layer

Jisun Kim[1], Hyoungdo Nam[2], Guorong Li[1], A. B. Karki[1], Zhen Wang[1,3], Yimei Zhu[3], Chih-Kang Shih[2], Jiandi Zhang[1], Rongying Jin[1], and E. W. Plummer[1]

[1]Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803, USA

[2]Department of Physics, The University of Texas, Austin, TX 78712, USA

[3]Brookhaven National Laboratory, Upton, NY 11973, USA

9:40 a.m. – 10:00 a.m. Coffee Break (RCED atrium)

Session 2 Moderator: Prof. Jak Chakhalian, University of Arkansas

10:00 a.m. – 10:20 a.m.

Revealing Previously Unknown Intracellular Organization of Bacterial Plasmids using Super-Resolution Microscopy

Y. Wang[1], P. Penkul[2], J. N. Milstein[2]

[1]Department of Physics, University of Arkansas, 825 Dickson St, Fayetteville, AR, 72701, USA

[2]Department of Physics, Department of Chemical & Physical Sciences, University of Toronto, ON, Canada

10:20 a.m. – 10:40 a.m.

The 2D Selfassembly of Benzimidazole and its Co-crystallization

P. S. Costa[1], D. Miller[2], J. Teeter,[3] James Hooper, S. Beniwal, A. Sinitskii, E. Zurek, and A. Enders[2]

[1]Department of Physics and Astronomy, University of Nebraska-Lincoln, Lincoln, NE 68588, USA

[2]Department of Chemistry, State University of New York at Buffalo, Buffalo New York 14260-3000, USA

[3]Department of Chemistry, University of Nebraska-Lincoln, Lincoln, NE 68588, USA

[4]Department of Theoretical Chemistry, Faculty of Chemistry, Jagiellonian Univeristy, 30-060 Krakow, Poland

10:40 a.m. – 11:00 a.m.

Formation of bulk-like, two-dimensional CuSe on Cu(111) at ultra-low selenium coverage

P.A. Thiel[1,2,3], Holly Walen,[1,4] Da-Jiang Liu,[2] Junepyo Oh,[4] Hyun Jin Yang,[4] and Yousoo Kim[4]

[1]Department of Chemistry, Iowa State University, Ames, IA 50011
[2]Ames Laboratory, Ames, IA 50011
[3]Department of Materials Science & Engineering, Iowa State University, Ames, IA
[4]Surface and Interface Science Laboratory RIKEN, Wako, Saitama 351-0198 Japan

11:00 a.m. – 11:20 a.m.

Avoiding polar catastrophe in materials with high polar mismatch $LaNiO_3/SrTiO_3(111)$*

M. Saghayezhian, Z. Wang , H. Guo, J. Zhang, and E.W. Plummer
Department of Physics, Louisiana State University, Baton Rouge, LA, 70803, USA

11:20 a.m. – 12:00 p.m.

INVITED TALK:

New Device Frontiers for Electronic Nano-Materials

Jochen Mannhart
Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany

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12:00 p.m. – 1:00 p.m. Lunch (RCED 103-107)

Session 3 Moderator: Prof. Jiali Li, University of Arkansas

1:00 p.m. – 1:20 p.m.

Understanding the Role of Electrons in Chemical Bond Breaking and Phase Transition

B. Wang
School of Chemical, Biological and Materials Engineering, University of Oklahoma, Norman, OK, 73019, USA

1:20 p.m. – 1:40 p.m.

Assembly and stability of metallic nanoclusters on metal(100) surfaces: Predictive atomistic modeling with ab-initio kinetics

Jim Evans[1], Patricia Thiel[2], and Yong Han[1]
[1]Department of Physics & Astronomy, Iowa State University, Ames, IA, 50011, USA
[2]Department of Chemistry, Iowa State University, Ames, IA, 50011, USA

1:40 p.m. – 2:00 p.m.

Spin-Lattice Coupling: the Essence in Magnetoelectric Digital Superlattices

Hangwen Guo[1], Zhen Wang[1,2], Shuai Dong[3], Mohammad Saghayezhian[1], Lina Chen[1], Rongying Jin[1], Yimei Zhu[2], Jiandi Zhang[1] and E. W. Plummer[1]

[1]Department of Physical and Astronomy, Louisiana State University, Tower Dr., Baton Rouge, LA, 70803, USA

[2]Department of Energy Science and Technology, Brookhaven National Laboratory, Upton, NY, 11973, USA

3Department of Physics, Southeast University, Nanjing, Jiangsu, 211189, China

2:00 p.m. – 2:40 p.m.

INVITED TALK:

Ferroelectric-based heterostructures

S. Boyn, A. Sander, R. O. Cherifi, A. Chanthbouala, L. Phillips, V. Ivanovskaya, H. Yamada, V. Garcia, S. Fusil, C. Carretero, J. Grollier , M. Bibes, A. Barthélémy

Unité Mixte de Physique CNRS / Thales, 1 av. Fresnel, 91767 Palaiseau & Université Paris-Sud, 91405 Orsay , France

B. Dkhil

Laboratoire SPMS, ECP, Grande voie des vignes, 92290 Châtenay-Malabry, France

A. Zobelli, A. Gloter

Laboratoire de Physique des Solides, Université Paris-Sud, 91405 Orsay, France

S. Valencia

Helmholtz Zentrum Berlin für Materialen und Energie, Albert-Einstein-Strasse 15, 12489 Berlin, Germany

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2:40 p.m. – 3:00 p.m. Coffee Break (RCED atrium)

3:00 p.m. – 5:00 p.m. Poster Session (RCED 111)

Poster 1

Cholesterol Influence on Arginine-Containing Transmembrane Peptides

Jordana K. Thibado[1], Ashley N. Martfeld[1], Denise V. Greathouse[1], Roger E. Koeppe II[1]

[1]Department of Chemistry and Biochemistry, University of Arkansas, Fayetteville, AR, 72701, USA

Poster 2

Determination of the Effect of Maillard Products on the Taxonomic Composition on the Gut Microbiota

ALJahdali N.,[1*]Gadonna P.,[2] Anton-Gay P.,[2] Carbonero F.[1,3]

[1]Cellular and Microbiology Program; University of Arkansas, AR, USA

[2]Expression des Gènes et régulation Epigénétique par l'Aliment; Institut Polytechnique LaSalle, Beauvais, France

[3]Department of Food Science; University of Arkansas, AR, USA

Poster 3

Synthesis and characterization of nickel oxide thin film and nanoparticles for hole transport in an all-inorganic colloidal quantum dot LED

R. Vasan [1], H. Salman2, and M. O. Manasreh[1]

[1]Department of Electrical Engineering, University of Arkansas, Fayetteville, AR, USA-72701

[2]Microelectronics and Photonics program, University of Arkansas, Fayetteville, AR, USA-72701

Poster 4

Measuring functional implications of inhomogeneous Acetylcholine distribution in cerebral cortex

T. Nur[1], S. H. Gautam[2], J. A. Stenken[3] and W. L. Shew[2]

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[3]Department of Chemistry & Biochemistry, University of Arkansas, 1 University of Arkansas, Fayetteville, AR, 72701, USA

Poster 5

Revealing Bacterial Responses to Environmental Changes using Super-Resolution Microscopy

Sai Divya Challapalli[1] and Yong Wang[2]

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[2]Department of Physics, University of Arkansas, 825 W. Dickson St. Fayetteville, AR 72701

Poster 6

Understanding electron energy loss mechanisms in EUV resists using photoemission and electron energy loss spectroscopies

James P. Horwath[1], Sylvie Rangan[1], Robert Allen Bartynski[1], Amrit Narasimhan[2], Robert Brainard[2] and Mark Neisser[3]

[1]Department of Physics and Astronomy, Rutgers University, 136 Frelinghuysen, Piscataway, NJ, USA

[2]SUNY Polytechnic Institute, College of Nanoscale Science and Engineering, 257 Fuller, Albany, NY, USA

[3]SUNY Polytechnic Institute SEMATECH, 257 Fuller Road, Albany, 12203 NY, USA

Poster 7

Measuring Nonlinear properties of Graphene Thin Films Using Z-Scan Technique

A. AlAbdulaal[1] and G. Salamo[1]

[1]Microelectronics Photonics Program, Department of Physics, Institute for Nanoscience and Engineering, University of Arkansas, Fayetteville, AR 72701, USA

Poster 8

Transport Properties of Cobalt Doped ZnO/p-Si Heterojunction Using Impedance Analysis and Exciton Lifetime Measurement

A. Kaphle[1], R. Tiwari[1] and P. Hari[1]

[1]Department of Physics, University of Tulsa, 800 S Tucker Dr, Tulsa, OK, 74104, USA.

Poster 9

Direct Two-photon Absorption Induced Emission of InAs/GaAs Quantum dots

X.Hu[1,2], D.Guzun[2], M.E.Ware[2,3], Yu.I.Mazur[2], G.J.Salamo[1,2]

[1]Department of Physics, University of Arkansas, 825 W. Dickson St., Fayetteville, AR, 72701, USA

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[3]Department of Electrical Engineering, University of Arkansas, Bell Engineering, Fayetteville, AR, USA

Poster 10

Investigation the conditions of the conformal shell layers formed by different types of PVD techniques on different aspect ratio nanorods arrays.

M. Yurukcu[1], H. Cansizoglu[2] , F. Cansizoglu[3] and T. Karabacak[1]

[1]*Department of Physics and Astronomy, University of Arkansas at Little Rock, Little Rock, AR, 72211, United States*

[2]*Department of Electrical and Computer Engineering, University of California, Davis, CA, 95616, United States*

[3]*Green Center for Systems Biology, University of Texas Southwestern Medical Center, Forest Park,Dallas, TX, 75390, United States*

Poster 11

Dual-width plasmonic gratings with tunable optical enhancement for Raman spectroscopy substrates

S. J. Bauman[1], A. A. Darweesh[1], G. P. Abbey[2], A. M. Hill[3], and J. B. Herzog[3]

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[3]Department of Physics, University of Arkansas, 825 W. Dickson St., Fayetteville, AR, 72701, USA

Poster 12

Digitization and Additive Manufacturing of Natural Surfaces

M. Afshar-Mohajer[1], M. Zou[1]

[1]Department of Mechanical Engineering, University of Arkansas, Fayetteville, AR, 72701, USA

Poster 13

Photoluminescence study of InN/GaN multi-quantum well under biaxial strain

Y. Wu,[1] C. Li,[1] A. Kuchuk,[1] M. E. Ware[2] and G. Salamo[3]

[1]Microelectronics and Photonics Program, University of Arkansas, Fayetteville, AR 72701, USA

[2]Department of Electrical Engineering, University of Arkansas, Fayetteville, AR 72701, USA

[3]Department of Physics, University of Arkansas, Fayetteville, AR 72701, USA

Poster 14

ELECTROCHEMICAL-STM INVESTIGATION OF SILVER HALIDE MONOLAYERS ON A AU(111) SURFACE

J.A. Phillips[1], L. Jackson, H. Morgan, G. Jones, E.V. Iski[1] and S. Wang[2]

[1]Department of Chemistry and Biochemistry, University of Tulsa, 800 S. Tucker Dr., Tulsa, OK, USA

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Poster 15

Surface Texturing for Friction Reduction via 3D Printing

R. Araujo Borges[1] and M. Zou[1]

[1]Department of Mechanical Engineering, University of Arkansas, 863 West Dickson Street, Fayetteville, AR, 72701, USA

Poster 16

The nature of metal-insulator transition in ultrathin $SrVO_3$ films*

Gaomin Wang[1], Zhen Wang[2], Chen Chen[1], Mohammad Saghayezhian[1], Lina Chen[1], Hangwen Guo[1], Yimei Zhu[2], Ward Plummer[1] and Jiandi Zhang[2]

[1]Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA, 70803, USA

[2]Brookhaven National Laboratory, Upton, NY, 11973, USA

Poster 17

Engineered Surfaces with Deformation-Resistant Core-Shell Nanostructures

R. Fleming[1,2] and M. Zou[1,2]

[1]Department of Mechanical Engineering, University of Arkansas, Fayetteville, AR, 72701, USA

[2]Center for Advanced Surface Engineering, University of Arkansas, Fayetteville, AR, 72701, USA

Poster 18

$SrRuO_3$ (111) thin films with persistent $(\sqrt{3} \times \sqrt{3})R30°$ surface reconstruction*

Weimei Xie[1, 2], M. Saghayezhian[2], X.M. Gu[1], Hangwen Guo[2], Chen Chen[2], X.S. Wu[1], E.W. Plummer[2] and Jiandi Zhang[2]

[1] Collaborative Innovation Center of Advanced Microstructures, Lab of Solid State Microstructures, School of Physics, Nanjing University, Nanjing 210093, China

[2] Dept. of Physics & Astronomy, Louisiana State University, Baton Rouge, LA 70803, USA

Poster 19

Surface structural phase transition of IrTe2 studied by LEED

Yifan Yang, Chen Chen, Guixin Cao, Rongying Jin, E. W. Plummer
Department of Physics & Astronomy, Louisiana State University, Baton Rouge, Louisiana, USA

Poster 20

Bias-dependent rotation of thiol-tethered molecules on Au(111)

L. Ríos*, J. Lee, N. Tallarida and V. Ara Apkarian
Department of Chemistry, University of California Irvine, 1120 Natural Sciences, Irvine, CA, USA

Poster 21

Real-Space Analysis of Scanning Tunneling Microscope Images: Accurate measurements of local structure and disorder

Mitchell P. Yothers and Lloyd A. Bumm
Homer L. Dodge Department of Physics & Astronomy, The University of Oklahoma, Norman, OK, USA

Poster 22

Local Dynamics and Disorder of the Terminal Methyl Groups in *n*-Alkanethiol Self-Assembled Monolayers on Au(111): A molecular dynamics study

S. Bhattacharya[1], L. Huang[2], and L. A. Bumm[1]
[1]Homer L. Dodge Department of Physics & Astronomy, The University of Oklahoma, 440 W. Brooks St., Norman, OK 73019, USA
[2]School of Chemical, Biological and Materials Engineering, The University of Oklahoma, 100 E. Boyd St., Norman, OK 73019, USA

Poster 23

Exploring Macro Porous Silicon as a Substrate for Heterojunction Solar Cells

N. Shahabi Sani, Y. Cheng, N. Kantack, V.R. Whiteside, I. R. Sellers, and L. A. Bumm
Homer L. Dodge Department of Physics & Astronomy, The University of Oklahoma, 440 W. Brooks St., Norman, OK 73019, USA

Poster 24

Electronic states and optical transitions in the semiconductor layered biconical quantum dot

A. A. Tshantshapanyan, K. G. Dvoyan and B. Vlahovic
Department of Mathematics and Physics, North Carolina Central University, 1801 Fayetteville St., Durham, NC 27707, USA

Poster 25

Vertical electrical field induced monolayer island growth on $TiSe_2$

H. Zheng[1], S. Valtierra[2], N. Opoku[2], C. Chen[1], L. Jiao[3], K. Bevan[2], and C. Tao[1]
[1]Department of Physics, Virginia Tech, Blacksburg, Virginia 24061, USA
[2]Materials Engineering, McGill University, Montreal, H3A 0C5, Canada
[3]Department of Chemistry, Tsinghua University, Beijing 100084, China

Poster 26

Ordering of Organics on (111) Coinage Metals: Substrates Matter

Andrew S. DeLoach[1], Brad R. Conrad[2], T.L. Einstein[3], L. Bartels[4], & Daniel B. Dougherty[1]

[1]Department of Physics, North Carolina State University, Raleigh, NC 27695-8202 USA
[2]Department of Physics and Astronomy, Appalachian State University, Boone, NC 28608
[3]Department of Physics & CMTC, University of Maryland, College Park, MD 20742-4111
[4]Department of Chemistry, University of California at Riverside, Riverside, California 92521

Poster 27

Electronic States and the Size-Quantized Stark Effect in the Semiconductor Semi-Ellipsoidal Quantum Dot

K. G. Dvoyan[1], A. A. Tshantshapanyan[1], B. Vlahovic[1] and G. J. Salamo[2]

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[2]Institute for Nanoscience and Engineering, University of Arkansas, 731 West Dickson St., Fayetteville, AR 72701, USA

Poster 28

Surface Transport Study of Doped Ultra-Thin Sb Quantum Wells

K. S. Wickramasinghe, S. Cairns, J. Massengale, Z. Liu, C. K. Gaspe, T. D. Mishima, J. C. Keay, M. B. Johnson, S. Q. Murphy, and M. B. Santos

Homer L. Dodge Department of Physics and Astronomy, University of Oklahoma, 440 W. Brooks St., Norman, OK 73019, USA

Poster 29

First Principles Calculations of Charge Density Waves in 2H-$TaSe_2$: Dependence on Layer Number and Temperature

Sugata Chowdhury[1, 2], J.R. Simpson[1, 3], T.L. Einstein[4], A.R. Hight Walker[1]

[1]National Institute of Standards and Technology Gaithersburg, MD;
[2]Catholic University of America, Washington, DC; [3]Towson University, Towson, MD; [4]University of Maryland, College Park, MD

5:00 p.m. – 6:00 p.m.	Break before Picnic, PEC General Committee Meeting (RCED 232)
6:00 p.m. – 8:00 p.m.	Picnic at Hawkins Family Terrace

Wednesday, June 22, 2016

7:00 a.m. – 8:00 a.m. Breakfast – Reynolds Center (RCED 103-107)
Registration (all day) – Reynolds Center (RCED atrium)

Session 4 Moderator: Prof. Arun Nair, University of Arkansas

8:00 a.m. – 8:20 a.m.

Sensing the binding sites of RNAP Holoenzyme on λ phage DNA attached to a probe tip with Solid State Nanopores

H.Kaur* and J. Li

***Nottingham Contestant**

[1]Department of Physics, University of Arkansas, 825 W Dickson Street, Fayetteville, AR, 72701, USA

8:20 a.m. – 8:40 a.m.

Atomically Precise Design, Synthesis, and Characterization of 2D Material Interfaces

B. Kiraly[1,2]*, M. C. Hersam[1,3], N. P. Guisinger[2]

***Nottingham Contestant**

[1] Department of Materials Science and Engineering, Northwestern University, Evanston, Illinois 60208, USA

[2] Center for Nanoscale Materials, Argonne National Laboratory, Argonne, Illinois 60439, United States

[3] Department of Chemistry, Northwestern University, Evanston, Illinois 60208, United States

8:40 a.m. – 9:00 a.m.

Xe Irradiation of Graphene on Ir(111): From Trapping to Blistering

C. Herbig* and T. Michely

***Nottingham Contestant**

[1]II. Physikalisches Institut, University of Cologne, Zuelpicher Str. 77, Cologne, 50937, Germany

9:00 a.m. – 9:20 a.m.

Interfacial Engineering of Electronic and Magnetic States in Complex Oxide Heterostructures by Pulsed Laser Deposition Technique

Xiaoran Liu* and J. Chakhalian

***Nottingham Contestant**

[1]Department of Physics, University of Arkansas, 825 W. Dickson Street, Fayetteville, AR 72701, USA

9:20 a.m. – 9:40 a.m.

Electronic structure and first order structural transition of $LuFeO_3$

Shi Cao* and Peter Dowben

***Nottingham Contestant**

[1]Department of Physics and Astronomy, Nebraska Center for Materials and Nanoscience University of Nebraska-Lincoln, Lincoln, NE 68588, USA

9:40 a.m. – 10:00 a.m. Coffee Break (RCED atrium)

Session 5 Moderator: Prof. Paul Thibado, University of Arkansas

10:00 a.m. – 10:20 a.m.

Hidden Phases of Double-layered $Sr_3(Ru_{1-x}Mn_x)_2O_7$ Exposed at the Surface

Chen Chen* and E. W. Plummer

***Nottingham Contestant**

[1]Department of Physical and Astronomy, Louisiana State University, Tower Dr., Baton Rouge, LA, 70803, USA

10:20 a.m. – 10:40 a.m.

Electronic Phase Control in Electrolyte-Gated Correlated Oxides

Y. Zhou*[1] and S. Ramanthan[1,2]

***Nottingham Contestant**

[1]John A. Paulson School of Engineering and Applied Sciences, Harvard University, Cambridge, MA 02138, USA.

[2] School of Materials Engineering, Purdue University, West Lafayette, IN 47907, USA.

10:40 a.m. – 11:00 a.m.

Effect of Ligand Exchange with Mercaptoacetic Acid on the Photoresponsivity of Near-IR Photodetectors Based on PbSe Nanocrystals

Ahmad Nusir* and Omar Manasreh

***Nottingham Contestant**

Department of Electrical Engineering, University of Arkansas, Fayetteville, AR 72701, USA

11:00 a.m. – 11:20 a.m.

Exploring Intermolecular Interactions by Imaging Single Bonds with the Scanning Tunneling Microscope

Zhumin Han[1]* and Wilson Ho[1,2]

***Nottingham Contestant**

[1]Department of Physics and Astronomy, University of California, Irvine, California 92697-4575

[2]Department of Chemistry, University of California, Irvine, California 92697-2025

11:20 a.m. – 12:00 p.m.
INVITED TALK:
Mechanical engineering considerations for advanced application CPUs
Jonathan W. Thibado
PMCI Manager, Principal Engineer, Intel Corporation

12:00 p.m. – 1:00 p.m. Lunch (RCED 103-107)

Session 6 Moderator: Prof. Omar Manasreh, University of Arkansas

1:00 p.m. – 1:20 p.m.
Core level shifts of doped graphene
U. A. Schröder* and T. Michely
***Nottingham Contestant**
Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany

1:20 p.m. – 1:40 p.m.
Coupling Organic Molecules to Topological Insulators
Andy S. Hewitt* and Daniel B. Dougherty
***Nottingham Contestant**
Department of Physics, University of North Carolina State University, Raleigh, NC, 27606, USA

1:40 p.m. – 2:00 p.m.
Surface Reactivity of Pt-Cu(111) Single Atom Alloys:
Model Studies that Guide the Design of Atom Efficient Pt Nanoparticle Catalysis
F. R. Lucci* and E. C. H. Sykes
***Nottingham Contestant**
Department of Chemistry, Tufts University, 62 Talbot Avenue, Medford, MA, 02155 USA

2:00 p.m. – 2:20 p.m.
Synthesis and Characterization of MoS_2 thin films by Pulsed Laser Deposition for Electronic Applications
Martha I. Serna*[†,] Seong H. Yoo[‡], Thesis adviser: Manuel A. Quevedo-Lopez[†]
*Nottingham Contestant
[1]Materials Science and Engineering Department, The University of Texas at Dallas, Richardson, TX. USA
[2]Department of Advanced Materials Engineering, Kookmin University, Seoul, Korea
[3]Mechanical Engineering Department, The University of Texas at Dallas, Richardson,TX. USA
[4]Core Labs, King Abdullah University of Science and Technology (KAUST), Thuwal , Saudi Arabia

2:20 p.m. – 2:40 p.m.
Zinc(II) Tetraphenylporphyrin on Ag(100) and Ag(111): Multilayer Desorption and Dehydrogenation
C. Ruggieri* and R.A. Bartynski
***Nottingham Contestant**
Department of Physics and Astronomy, Rutgers, The State University of New Jersey, Piscataway, NJ 08854, USA

2:40 p.m. – 3:00 p.m. Coffee Break (RCED atrium)

Session 7 Moderator: Prof. Robert Coridan, University of Arkansas

3:00 p.m. – 3:20 p.m.
Electrical Control of Chiral Phases in Electrotoroidic Nanocomposites
R. Walter*[1,2] and L. Bellaiche[1]**
***Nottingham Contestant, **PhD Advisor to Contestant**
[1]Physics Department and Institute for Nanoscience and Engineering, University of Arkansas, Fayetteville, AR 72701
[2]Mathematics Department, University of Arkansas, Fayetteville, AR 72701

3:20 p.m. – 3:40 p.m.
Spin-Polarized Interfacial Hybridization between different 8-hydroxyquinolates and Cr(001) surface
J. Wang* and D. B. Dougherty
***Nottingham Contestant**
[1]Department of Physics, North Carolina State University, Raleigh, NC, 27695, USA

3:40 p.m. – 4:00 p.m.
Low-dimensional Organics for Electronics Applications
S. Beniwal* and A. Enders
***Nottingham Contestant**
Department of Physics & Astronomy, University of Nebraska, Lincoln, NE

4:00 p.m. – 4:20 p.m.
Van der Waals Epitaxy of WSe_2 Based Heterostructures: A Study of Controlled Nucleation and Grain Morphology
Ruoyu Yue* and Christopher Hinkle
***Nottingham Contestant**
Department of Materials Science and Engineering, University of Texas at Dallas, Richardson, TX 75080-3021, USA

4:20 p.m. – 4:40 p.m.
Layer-by-layer interrogation of $La_{2/3}Sr_{1/3}MnO_3$ films on $SrTiO_3$ (001)
Lina Chen* and Jiandi Zhang and E.W. Plummer
***Nottingham Contestant**
Department of Physics and Astronomy, Louisianan State University, Tower Dr. , Baton Rouge, La, 70803, USA

4:40 p.m. – 5:00 p.m.
Characterization of a gate-defined double quantum dot in a Si/SiGe nanomembrane
T. J. Knapp* and M. A. Eriksson
***Nottingham Contestant**
Wisconsin Institute for Quantum Information, University of Wisconsin—Madison, Madison, WI 53706-1390, USA

5:00 p.m. – 6:00 p.m.	Break before banquet, take down posters
6:00 p.m. – 8:00 p.m.	Banquet at Raymond Miller Hall of Champions
8:00 p.m. – 10:00 p.m.	Dickson Street Nottingham Prize Celebration

Thursday, June 23, 2016

6:30 a.m. – 8:00 a.m.	Check out of Maple Hill Dorms (take luggage to RCED)
7:00 a.m. – 8:00 a.m.	Breakfast – Reynolds Center (RCED 103-107)

Session 8 Moderator: Prof. Nicholas Materer, Oklahoma State University

8:00 a.m. – 8:20 a.m.
Synthesis of Two-Dimensional MoS_2 by a CVD Process
Yan Jiang*, Jingbiao Cui
Department of Physics and Materials Science, University of Memphis, 216 Manning Hall, Memphis, TN, 38152, USA

8:20 a.m. – 8:40 a.m.
Reaction of Dysprosium with Graphite Surface: Competition between Carbide Formation and Surface Intercalation
Ann Lii-Rosales[1,2], Yinghui Zhou[2,5], Mark Wallingford[2], Cai-Zhuang Wang[2,4], Michael Tringides[2,4], and P.A. Thiel[1,2,3]
[1]Department of Chemistry, Iowa State University, Ames, IA 50011, USA
[2]The Ames Laboratory, Ames, IA 50011, USA
[3]Deparment of Materials Science & Engineering, Iowa State University, Ames, IA 50011, USA
[4]Department of Physics & Astronomy, Iowa State University, Ames, IA 50011, USA
[5]Department of Physics, Xiamen University, Xiamen 361005, China

8:40 a.m. – 9:00 a.m.

Elucidating the mechanism of heterogeneous acetaldehyde oxidation on polycrystalline platinum through flow cell studies

S. C. Edington[1,*] and S. L. Bernasek[1]

[1]Department of Chemistry, Princeton University, Frick Laboratory, Washington Road, Princeton, NJ, 08544, USA

*Current address: Department of Chemistry, University of Texas at Austin, 102 E. 24th Street, Austin, TX, USA

9:00 a.m. – 9:20 a.m.

Adsorption of Ammonia and Water on Metal-supported Iron Phthalocyanine

Reda Bababrik, Bin Wang

Center for Interfacial Reaction Engineering and School of Chemical, Biological and Materials Engineering, the University of Oklahoma, Norman, 73019-1004 Oklahoma, USA

9:20 a.m. – 9:40 a.m.

Anomalously Deep Polarization in $SrTiO_3$(001) Interfaced with an Epitaxial Ultrathin Manganite Film*

Zhen Wang[1, 2], Jing Tao[2], Liping Yu[3], Hangwen Guo[1], Lina Chen[1], Myung-Geun Han[2], Lijun Wu[2], Huolin Xin[2], Kim Kisslinger[2], E. W. Plummer[1], Jiandi Zhang[1], and Yimei Zhu[2]

[1]Department of Physics & Astronomy, Louisiana State University, Baton Rouge, LA 70803

[2]Department of Energy Science and Technology, Brookhaven National Laboratory, Upton, NY

[3]Department of Physics, Temple University, Philadelphia, PA 19122

9:40 a.m. – 10:00 a.m. Coffee Break (RCED atrium)

Session 9 Moderator: Prof. Ryan Tian, University of Arkansas

10:00 a.m. – 10:20 a.m.

Titania Containing Thin Films for the Detection of TATP and Peroxide Vapors

Nicholas F. Materer[1], Travis H. James[1], Zeid AlOthman[2] and Allen Apblett[1]

[1]Department of Chemistry, Oklahoma State University, Stillwater, Oklahoma 74078-3071

[2]Chemistry Department, College of Science, King Saud University, Riyadh-11451, Kingdom of Saudi Arabia

10:20 a.m. – 10:40 a.m.

Epitaxial Growth of Graphene Nanoribbons on Cu(111)

J. Teeter[1], P. Costa[2], M. Pour[1], A. Enders[2], and A. Sinitskii[1]

[1]Department of Chemistry, University of Nebraska - Lincoln, Lincoln, Nebraska 68588, United States

[2]Department of Physics and Astronomy, University of Nebraska - Lincoln, Lincoln, Nebraska 68588, United States

10:40 a.m. – 11:00 a.m.

Enhanced Photoresponsivity by HIPS-GLAD and SAD-GLAD core/shell nanorod array photodetectors

F. Keles, H. Cansizoglu and T. Karabacak

Department of Physics and Astronomy, University of Arkansas at Little Rock, Little Rock, AR, 72204, USA

11:00 a.m. – 11:20 a.m.

The Manipulation and Analysis of ZnO Nanorods with Applications for Photovoltaic Devices

E. Adcock Smith[1], A. Kaphle[2], P. Hari[2] and K.P. Roberts[1]

[1] Department of Chemistry, University of Tulsa, 800 S. Tucker, Tulsa, Ok, 74104, USA

[2] Department of Physics, University of Tulsa, 800 S. Tucker, Tulsa, Ok, 74104, USA

11:20 a.m. – 11:30 a.m.	Closing Remarks
11:30 a.m. – 12:30 p.m.	Box Lunch (RCED 103-107)
12:00 p.m.	Free one-way shuttle to XNA, Crystal Bridges, 21C Hotel (last stop)

Session 1 notes:

Density Functional Theory Study of Chemical Functionalization of Two-dimensional Materials

Tong Mou [1], Bin Wang [1]

[1]School of Chemical, Biological and Materials Engineering, University of Oklahoma, Norman, Oklahoma, 73019, USA

Email: tong.mou-1@ou.edu

Graphene, as the first exfoliated two-dimensional (2D) material, has gained significant attention regarding its appealing electronic properties and potential applications in electronic devices, sensors and catalysis. Many of these properties rely on functionalization of the basal plane through surface modification. The interest has recently been extended to other two-dimensional materials that also show unique electronic and optical properties. In this study, we performed first-principles density functional theory (DFT) calculations to investigate chemical functionalization of monolayer graphene along with phosphorene, hexagonal boron nitride (h-BN) and molybdenum disulfide (MoS2) with phenyl and phenolate species. We examined their adsorption properties and relative stability through calculation of binding energies. Their electronic structures (density of states) were calculated in comparison with the pristine structures to reveal how these different functional groups modify their electronic properties. Our results indicated that chemical functionalization of all the materials with phenyl groups could be an effective influence on their electronic properties by introducing defect levels around the Fermi level and between the band gaps. Instead, only phosphorene is sensitive to the presence of phenolate, which could not be adsorbed on any other materials that we have tried. The results would help shed some light on the promising electronic properties of 2D materials for future device and sensor applications.

SAD-GLAD Pt-Ni @Ni nanorods as Highly Active Oxygen Reduction Reaction Electrocatalysts

Mahbuba Begum[1], Nancy N. Kariuki[2], Mehmet F. Cansizoglu[1], Mesut Yurukcu[1], Fatma M. Yurtsever[1], Tansel Karabacak[1], and Deborah J. Myers[2]

[1]Department of Physics and Astronomy, University of Arkansas at Little Rock, Little Rock AR 72204, USA

[2]Chemical Sciences and Engineering Division, Argonne National Laboratory, Argonne, IL 60439-4837, USA

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ABSTRACT: Vertically aligned catalysts comprised of platinum-nickel thin films on nickel nanorods (designated as Pt-Ni@Ni-NR) with varying ratios of Pt to Ni in the thin film were prepared by magnetron sputtering and evaluated for their oxygen reduction reaction (ORR) activity. A glancing angle deposition (GLAD) technique was used to fabricate the Ni nanorods (NRs) and a small angle deposition (SAD) technique for growth of a thin conformal coating of Pt-Ni on the Ni-NRs. The Pt-Ni@Ni-NR structures were deposited on glassy carbon for evaluation of their ORR activity in aqueous acidic electrolyte using the rotating disk electrode technique. The Pt-Ni@Ni-NR catalysts showed superior area-specific and mass activities for ORR compared to Pt-Ni alloy nanorod catalysts prepared using the GLAD technique and compared to conventional high-surface-area Pt and Pt-Ni alloy nanoparticle catalysts.

Spatially Resolved Scanning Tunneling Spectroscopy of Single Layer Steps on Si(100) Surfaces: Experiment and Simulation

X.Wang[1,2], P. Namboodiri[2], K.Li[2], X.Deng[2], and R.Silver[2]

[1]Chemical Physics Program, University of Maryland, College Park, MD, 20742, USA

[2]Engineering Physics Division, National Institute of Standard and Technology, 100 Bureau Dr, Gaithersburg, MD 20899, USA

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Advanced Hydrogen lithography enables the fabrication of atomically precise donor-based quantum devices on Si(100) surfaces. Understanding the defect and step edge interaction with local electronic and geometric structures is necessary to properly interpret device measurement results.

A spatially resolved scanning tunneling spectroscopy (STS) study was carried out across single layer SA and SB step edges on Si(100) surfaces at room temperature. The observed local density of states on flat Si(100) terraces agree very well with previous photoemission spectroscopy studies [1,2]. The local density of states (LDOS) across SA steps was found to be very similar to that on a flat terrace. Along the rebonded SB step edge, the presence of a finite-length of unpaired dangling bonds as well as the rebonding-induced charge redistribution significantly modifies the local electronic properties across the rebonded SB step edge. Metallic behavior is observed along the rebonded SB step edge based on local spectroscopic measurements. Electrostatic potential calculations permit us to evaluate tip and edge state parameters by fitting the calculated band bending with experimental observations. The charge states introduced by the rebonded SB step edge and its spatial effects are quantified using a uniform surface state distribution model, which also agrees well with a finite line of charge model.

This study will help to elucidate the role played by surface step edges and tip parameters in characterizing surface or sub-surface atomic structures using STS/STM.

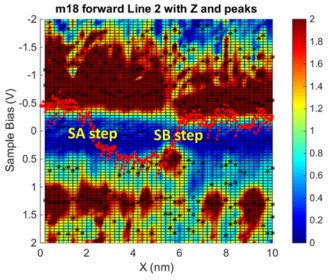

Fig. 1. The normalized differential conductance map across monolayer SA and SB step edges on Si(100) surface.

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[2] L. S. O. Johansson and B. Reihl, Surface Science 269, 810 (1992).

Interrogating the superconductor $Ca_{10}(Pt_4As_8)(Fe_{2-x}Pt_xAs_2)_5$ Layer-by-layer

Jisun Kim[1], Hyoungdo Nam[2], Guorong Li[1], A. B. Karki[1], Zhen Wang[1,3], Yimei Zhu[3], Chih-Kang Shih[2], Jiandi Zhang[1], Rongying Jin[1], and E. W. Plummer[1]

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Ever since the discovery of high-T_c superconductivity in layered cuprates, the roles that individual layers play have been debated, due to difficulty in layer-by-layer characterization. While there is similar challenge in many Fe-based layered superconductors, the newly-discovered $Ca_{10}(Pt_4As_8)(Fe_2As_2)_5$ provides opportunities to explore superconductivity layer by layer, because it contains both superconducting building blocks (Fe_2As_2 layers) and intermediate Pt_4As_8 layers. Cleaving a single crystal under ultra-high vacuum results in multiple terminations: an ordered Pt_4As_8 layer, two reconstructed Ca layers on the top of a Pt_4As_8 layer, and disordered Ca layer on the top of Fe_2As_2 layer. The electronic properties of individual layers are studied using scanning tunneling microscopy/spectroscopy (STM/S), which reveals different spectra for each surface, as shown in Fig. 1. Remarkably superconducting coherence peaks are seen only on the ordered Ca/Pt_4As_8 layer. Our results indicate that an ordered structure with proper charge balance is required in order to preserve superconductivity.

*Supported by NSF-DMR 1504226

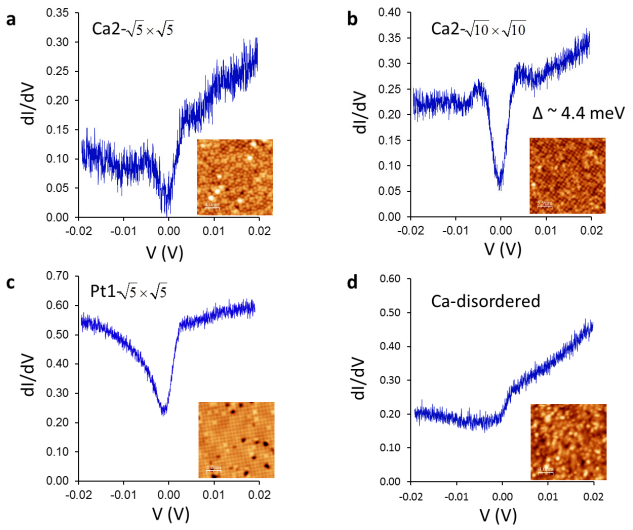

Fig. 1. STM images of four observed surfaces (inset) and spectra corresponding to each surface taken at 4.3 K: (**a**) Ca2-$\sqrt{5}\times\sqrt{5}$, (**b**) Ca2-$\sqrt{10}\times\sqrt{10}$, (**c**) Pt1-$\sqrt{5}\times\sqrt{5}$, and (**d**) Ca-disordered.

Session 2 notes:

Revealing Previously Unknown Intracellular Organization of Bacterial Plasmids using Super-Resolution Microscopy

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Plasmids play essential roles in bacterial metabolism, pathogenesis, and evolution, and are commonly engineered for recombinant protein synthesis and industrial fermentation. Deterring the persistence of harmful plasmids and enhancing the retention of beneficial ones require a better understanding of the fundamental mechanisms behind the maintenance of plasmids. The maintenance of high-copy number (hcn) plasmids relies significantly on how they are distributed spatially inside bacteria. Previous experiments using conventional light microscopy observed hcn plasmids clustering into discrete clusters, which seemed to raise issues on the maintenance of plasmids in bacteria over generations. We revisited the intracellular organization of hcn plasmids (a ColE1-derivative) in *E. coli* bacteria using an emerging powerful technique - quantitative super-resolution fluorescence microscopy based on single-molecule localization - with a resolution surpasses that of conventional light microscopy by ~10 to 20 fold. We observed that, although some hcn plasmids aggregated into large clusters, a majority of the plasmids were randomly distributed throughout the bacteria, minus an excluded volume of the nucleoid DNA of the bacteria. We also quantified the spatial distribution of plasmids in bacteria. Our results showed a "mixed distribution model" of both randomly diffusing plasmids and large clustered aggregates, which has not been observed previously. The observed “mixed model” may imply evolutionary importance, and hint possible approaches toward engineering the maintenance of hcn plasmids.

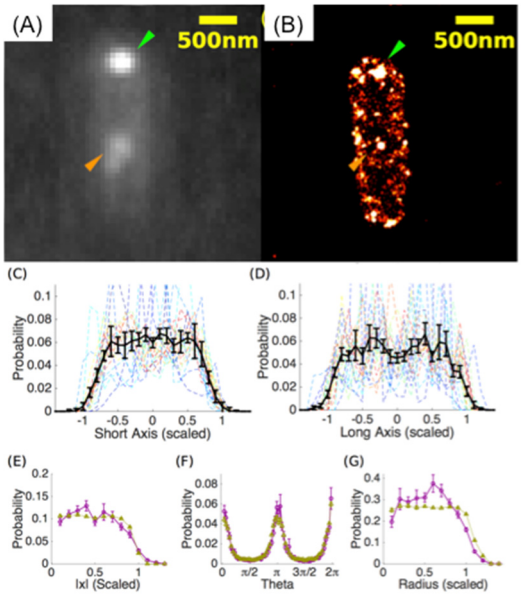

Fig. 1. Fluorescent images of hcn plasmids in a bacterium from (A) conventional light microscopy, or (B) super-resolution microscopy. (C-G) Quantification of the spatial distribution of plasmids in bacteria.

The 2D Selfassembly of Benzimidazole and its Co-crystallization

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Benzimidazoles (BI) are organic molecules that form crystals that are found to be room temperature ferroelectrics [1]. The origin of their ferroelectric behavior are the bistable N···HN bonds, and how they couple to the π electron distribution of the molecules. With both the molecular dipoles and the hydrogen bonds within the molecular plane a 3D crystal structure is not required for ferroelectricity to occur. Therefore, 2D and even 1D organic ferroelectrics based on these so-called proton transfer ferroelectric materials should be possible. We capitalized on surface-supported self-assembly to construct 1D and 2D structures of BI and croconic acid (CA). We observed with scanning tunneling microscopy that on Au and Ag surfaces, BI assembles into 1D zipper-like chains, which pack densely into a continuous 2D layer. DFT analysis confirms that the keto-enol forms that lead to ferroelectricity in the bulk also exist in the chains, and that the substrate actually lowers the energy barrier for proton transfer along the H-bond axis. In analogy, CA forms 2D sheets as well by forming O···HO – type H-bonds. This suggested the possibility to construct 2D co-crystals exhibiting heterogeneous OH···N bonds. On Au(111) CA and BI formed a co-crystal based on CA_2BI_2 tetramers as smallest building block. The tetramers bind together to form a 1D molecular chain, which exhibits both homogeneous OH···O bonds and heterogeneous NH···O bonds, suggesting that a hierarchy of switching barriers of the bonds must exist that might lead to the first multistate ferroelectrics.

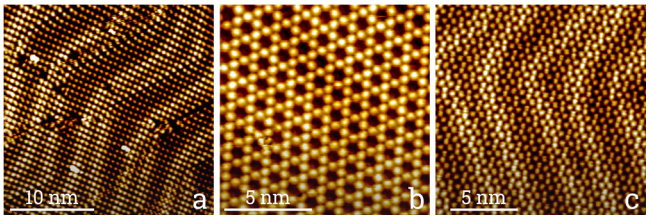

Fig. 1. STM images of molecules on Au(111) (a) BI, forming long chains; (b) CA, forming a honeycomb network; (c) BI and CA forming a co-crystal.

References:

[1] S. Horiuchi, et al. Nature com. **3**, 1308 (2012).

Formation of bulk-like, two-dimensional CuSe on Cu(111) at ultra-low selenium coverage

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Using scanning tunneling microscopy (STM), we observe that adsorption of Se on Cu(111) produces islands with (√3 x √3)R30° structure, at Se coverages of 0.02-0.06 monolayers. This is far below the structure's ideal coverage of 1/3 ML. Based on density functional theory (DFT), these islands cannot form due to attractive interactions between chemisorbed Se atoms. DFT shows that incorporating Cu atoms into the √3-Se lattice stabilizes the structure, which provides a plausible explanation for the experimental observations. STM reveals 3 types of √3 textures. We assign 2 of these as two-dimensional layers of strained CuSe, analogous to dense planes of bulk klockmannite (CuSe). Klockmannite has a bulk lattice constant 11% shorter than √3 times the surface lattice constant of Cu(111). This offers a rationale for these textures, where strain limits the island size or distorts the √3 lattice. Se stands in contrast to S, which forms small complexes with Cu under comparable conditions on Cu(111).[1,2] Possible reasons for this difference are discussed.

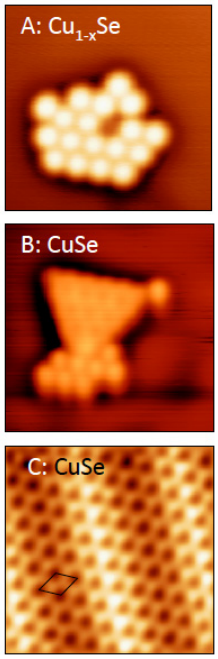

Figure (at right). Illustration of the three types of island textures observed with STM, after Se is deposited on Cu(111) at 300 K, then cooled to 5 K for imaging. Image sizes are 4 x 4 nm^2 in A and C, and 5 x 5 nm^2 in B.

References:

[1] **H. Walen, D.-J. Liu, J. Oh, H. Lim, J. W. Evans, C. Aikens, Y. Kim, P. A. Thiel, *Phys. Rev. B*. 91, 045426 (2015).**
[2] **H. Walen, D.-J. Liu, J. Oh, H. Lim, J. W. Evans, Y. Kim, P. A. Thiel, *J. Chem. Phys.* 142, 194711 (2015).**

Avoiding polar catastrophe in materials with high polar mismatch $LaNiO_3/SrTiO_3(111)$*

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Emergence of novel properties such as superconductivity, high mobility 2D electron gas and topological phases at the interface of oxide materials has proven the key role of interface engineering in material science. Interfaces in (111) direction have been predicted to show variety of intriguing properties such as topological interface state, Dirac half-metal phase and quantum anomalous Hall effect. So far, none of these predicted properties have been experimentally observed mainly due to high polarity of interface which leads to severe interface intermixture. To understand how to control the polarity at the interface, we studied the surface of $SrTiO_3$ (111). Using Low energy electron diffraction and X-ray photoemission spectroscopy we showed that there is a narrow temperature window that one can have a substrate with desired termination without any surface reconstruction (Figure 1). Our ability to control the polarity at the surface of $SrTiO_3$ (111) enabled us to grow $LaNiO_3/SrTiO_3$ (111) which has polar mismatch at interface, with sharp interface in the correct phase (Figure 2). This will open pathway to create interfaces with great quality at atomic scale in polar direction with polar mismatch. Using LEED and AR-XPS we will discuss the surface structure and electronic properties of $LaNiO_3/SrTiO_3$ (111) as a function of thickness.

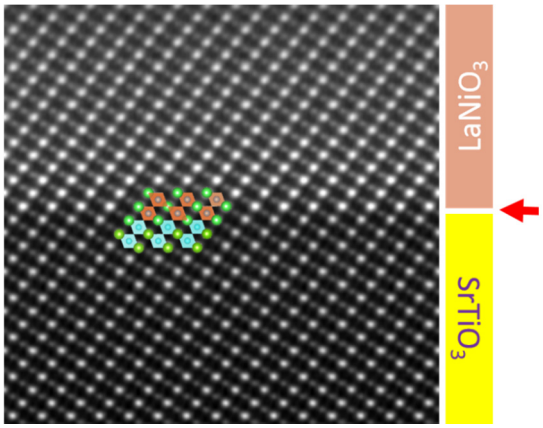

Figure 2 The TEM image of $LaNiO_3/SrTiO_3(111)$. The interface is well defined and there is no interface intermixture.

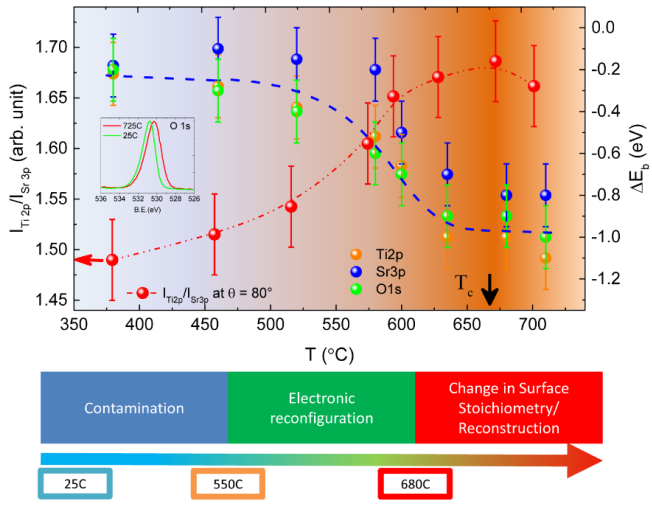

Figure 1(*top*). XPS core levels of Sr, Ti and O as a function of temperature. The drop in binding energy due to final state effect shows the presence of electron at the surface of $SrTiO_3$ (111). *(Bottom)* Polar compensation mechanism as a function of temperature.

*Mohammad Saghayezhian et al Phys. Rev. B **93** 125408 (2016).*

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No. DOE DE-SC0002136

INVITED TALK:

New Device Frontiers for Electronic Nano-Materials

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Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany

The phase space of electronic materials has been rapidly expanding, arguably beginning with germanium in the 1940s, to now include grapheme, related 2D materials, topological insulators, artificial 2D electron systems in complex oxides, and cold atoms, to give a few examples.

In this presentation I will discuss the potential of nano-materials to create novel and possibly useful electron systems, and will identify new frontiers for future nanoscale electronic devices.

Session 3 notes:

Understanding the Role of Electrons in Chemical Bond Breaking and Phase Transition

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The interplay among the microscopic degrees of freedom can generate macroscopic phenomena, such as reversible molecular switch and insulator-metal transition that have attracted long-standing interest for their potential applications in data storage and information processing. Here I will report our recent computational simulations of two different systems, through which the role of electrons on the chemical bond breaking and phase transition will be demonstrated. The first example is chemical functionalization of metal-supported graphene using iron phthalocyanine molecules. We show reversible control of the interfacial bonding between non-covalent and covalent interaction via electrical and thermal stimuli [1]. In the second example, I will focus on vanadium dioxide (VO_2), which shows a phase transition from a low-temperature semiconducting phase to a high-temperature metallic phase at 68°C with a rapid change in the electronic and optical properties. We find that the phase transition of VO_2 can be controlled by external photo stimuli in an Au/VO_2 hybrid material. Our calculations reveal the underlying physics of the phase transition and the role of the charge carriers on the phonons [2].

References:

[1] S. J. Altenburg, M. Lattelais, B. Wang, M.-L. Bocquet, R. Berndt, J. Am. Chem. Soc. **137** (29), 9452 (2015).

[2] K. Appavoo, B. Wang, N. F. Brady, M. Seo, J. Nag, R. P. Prasankumar, D. J. Hilton, S. T. Pantelides, R. F. Haglund, Nano Lett. **14**, 1127 (2014).

Assembly and stability of metallic nanoclusters on metal(100) surfaces: Predictive atomistic modeling with ab-initio kinetics

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Self-assembly of metal nanoclusters, either by deposition on smooth surfaces or in solution, often occurs far-from-equilibrium. Shape and structure depend of the fine details of relaxation kinetics in the aggregated state. Predictive modeling for epitaxial nanoclusters thus requires precise determination of barriers for periphery diffusion and intermixing for many possible local environments. We have developed a strategy to determine these barriers at the level of ab-initio DFT. This requires evaluation of interactions between adatoms not just conventionally at hollow adsorption sites, but also at bridge sites (the transition state for adatom diffusive hopping). These barriers provide the input for stochastic atomistic models analyzed by KMC simulation.

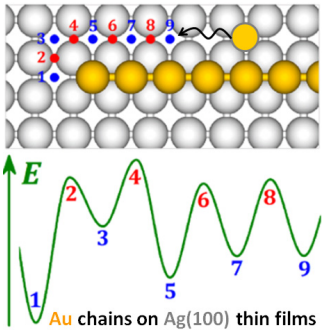

Fig.1. Formation of Au chains on Ag(100) films.

Our modeling is applied to self-assembly during deposition where quasi-equilibrated near-square islands are expected on metal(100) surfaces due to facile edge diffusion. This applies for Ag/Ag(100) and Au/Ag(100) at 300K, although bimetallic (Au+Ag)/Ag(100) islands formed by sequential co-deposition exhibit non-equilibrium core-ring structure [1]. Also, for Au/Ag(100) at 250K, we find the formation of atomic chains (Fig.1) induced by strong linear trio attractions and enhanced by quantum size effects [2].

Our modeling also applies for post-deposition coarsening of nanocluster arrays which is generally dominated by island diffusion and coalescence on metal(100) surfaces. Our modeling can precisely recover the time-scale (which depends on size) and shape evolution during the coalescence process [2,3]. See Fig.2.

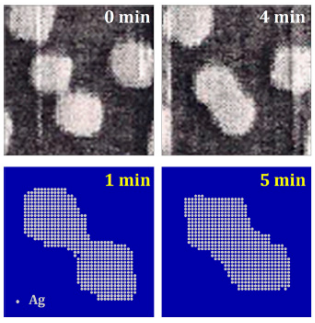

Fig.2. Coalescence of Ag nanoclusters on Ag(100).

References:

[1] Y. Han, D.-J. Liu, J.W. Evans, NanoLett. **14**, 4646 (2014).

[2] Y. Han, J.W. Evans, J. Phys. Chem. Lett. **6**, 2194 (2015).

[3] Y. Han, C.R. Stoldt, P.A. Thiel, J.W. Evans, in preparation.

Work supported by NSF Grants CHE-1111500 and CHE-1507223.

Spin-Lattice Coupling: the Essence in Magnetoelectric Digital Superlattices

Hangwen Guo[1], Zhen Wang[1,2], Shuai Dong[3], Mohammad Saghayezhian[1], Lina Chen[1], Rongying Jin[1], Yimei Zhu[2], Jiandi Zhang[1] and E. W. Plummer[1]

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Understanding magnetoelectric coupling in oxide heterostructures requires exploring the nature of their interface with atomic precision. In this work, we present direct evidence of structure induced unusual magnetism in these systems. By fabricating digital superlattices consist of ferroelectric $BaTiO_3$ (BTO) & ferromagnetic $La_{2/3}Sr_{1/3}MnO_3$ (LSMO) with extremely sharp interfaces and using atomically resolved scanning transmission electron microscopy (STEM), we reveal a thickness-dependent structural modulation in LSMO due to interfacial coupling with BTO, as shown in Fig.1. Such structural modulation leads to large change of ferromagnetism in LSMO and an abnormal reentrance of ferromagnetism in ultrathin regime. Our results highlight the importance of structural-property relationship in understanding the coupling effects in oxide heterostructures.

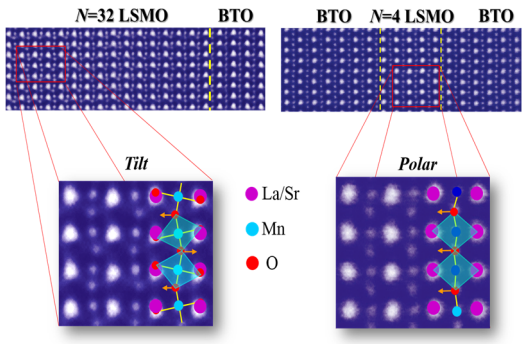

Fig. 1. High resolution annular bright field STEM image along [110] direction, for 32 unit cell (uc) & 4 unit cell LSMO, both sandwiched by BTO. Distinct structure change of LSMO is resolved from conventional tilt (32uc) to unconventional polar (4uc).

* Supported by U.S. DOE under Grant No. DOE DE-SC0002136.

INVITED TALK:

Ferroelectric-based heterostructures

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Ferroelectric materials possess a spontaneous polarization that can be switched by an external electric field and used to modulate the properties of an adjacent layer. To study this opportunity, we combined ferroelectric materials ($BaTiO_3$, $BiFeO_3$ in tetragonal phase) with the Mott insulator $(Ca,Ce)MnO_3$ (CCMO) and the transition metal alloy FeRh.

We studied Ferroelectric tunnel junctions (FTJs) composed of an ultrathin ferroelectric tunnel barrier. In junctions of T-BFO sandwiched between a CCMO and a Co/Pt counter-electrode, the tunneling current significantly depends on the orientation of the ferroelectric polarization, resulting in large electroresistance enabling a simple non-destructive readout of the ferroelectric state [1]. They exhibit fast, stable, multistate switching with very high resistance ratios of up to four orders of magnitude and very good endurance and retention characteristics of interest for future memristive devices [2]. Combined piezoresponse force microscopy (PFM) and electrical measurements give a clear correlation between ferroelectric domain configurations and multiple resistance states; they also provide insights into the switching dynamics in response to trains of nanosecond pulses. These FTJs also open the opportunity to tune the spin polarization of the Co or Fe counter-electrode by polarization reversal resulting in an electric control of the Tunnel Magnetoresistance observed in magnetic tunnel junctions [3].

In a field effect geometry, we observed that upon polarization reversal of the T-BFO ferroelectric gate, a CMO channel exhibits a non-volatile resistance switching by a factor of 4 around room temperature, and up to a factor of 10 at 200 K[4]. Combining FeRh with $BaTiO_3$ substrates, we evidenced through X-ray diffraction and various magnetometry experiments that a giant, low-voltage control of the magnetism of FeRh can be obtained. This control results from the strain effect exerted on FeRh during the polarization reversal of $BaTiO_3$ [5].

[1] Nature 460, 81 (2009)
[2] ACS Nano 7, 5385 (2013); APL 104, 052909 (2014)
[3] Science 327, 1106 (2010) ; Nature Materials 10, 753 (2011)
[4] Scientific Reports 3, 2834 (2014)
[5] Nature Materials 13, 345 (2014); Sci Rep. 5: 10026 (2015)

Poster notes:

Poster 1

Cholesterol Influence on Arginine-Containing Transmembrane Peptides

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An essential component of animal cells, cholesterol exerts significant influence on the physical properties of the membrane and in turn, its constituents. One such constituent, the membrane protein, often contains polar amino acids. Although sparse, polar residues are highly conserved and play pivotal roles in determining specific structural and functional properties. To gain greater understanding of the membrane, and more broadly, cellular function, a model peptide framework termed "GWALP23" (acetyl-GGALWLALALAL^{12}AL^{14}ALALWLAGA-amide) is useful. Designed and created at the University of Arkansas, the peptide is composed of amino acid residues of glycine (G), alanine (A) leucine (L) and tryptophan (W). The limited dynamic averaging of NMR observables such as the deuterium quadrupolar splittings of labeled alanine residues makes GWALP23 favorable for single residue replacements. Previously, GWALP23 family peptides were characterized with single Leu to Arg mutations at positions 12 and 14 in single-lipid membranes.[1] GWALP23-R14 adopts a defined tilted orientation in DOPC bilayers, whereas GWALP23-R12 displays multi-state behavior. The goal of this research is to further characterize these peptides in cholesterol-containing bilayers. Specific deuterium-labeled alanine residues were incorporated into the R12 and R14 sequences to identify transmembrane peptide orientation by means of solid-state deuterium NMR. Both peptides were incorporated into phospholipid bilayers with varying cholesterol content (0%, 10%, or 20%). Our findings suggest that 10% or 20% cholesterol content has minimal impact on the orientation of the GWALP23-R14 peptide. (Although the NMR signals are broader and weaker in the presence of 20% cholesterol, the deuterium quadrupolar splittings for ^{2}H-Ala residues in GWALP23-R14 change little.) Conversely, cholesterol appears to reduce the multi-state behavior of GWALP23-R12, favoring a single transmembrane state for the helix. With 10% or 20% cholesterol content, the spectra exhibit defined quadrupolar splittings, suggesting that GWALP23-R12 adopts a predominant, tilted orientation in the presence of cholesterol. These results convey a conditional sensitivity of a complex multi-state peptide helix to the presence of cholesterol.

References:

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Poster 2

Determination of the Effect of Maillard Products on the Taxonomic Composition on the Gut Microbiota

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[1]Cellular and Microbiology Program; University of Arkansas, AR, USA

[2]Expression des Gènes et régulation Epigénétique par l'Aliment; Institut Polytechnique LaSalle, Beauvais, France

[3]Department of Food Science; University of Arkansas, AR, USA

Maillard reaction products (MRPs) are the chemical reactions between amino acids and reducing sugar generated after the heat treatment of food. It has been reported that highly heated pellets, mice food, were proved to significantly protect against inflammation of experimental colitis in mice. The aim of this study is to determine the effect of Maillard products on the taxonomic composition of gut microbiota in mouse models of digestive diseases. In this study mice were divided into 3 groups and given chow subjected to various heat treatments (no treatment (control), moderately heated 121 ° C for 30 min, and highly heated 150 ° C for 15 min. The fecal samples were collected and microbial DNA extracted. Illumina MiSeq sequencing was used to survey the gut microbiota by targeting the V4 region of the bacterial 16S rRNA gene. In general, microbial communities were dominated by phylum level of *Firmicutes* and *Bacteroidetes*. Sequences were analyzed with the Basespace software and Mothur. Highly heated maillard products consumption resulted in a very significant increase of Firmicutes, specifically *Blautia* and *Faecalibacterium* spp. This increase was mainly at the expense of *Bacteroides* spp. The consumption of moderately had more moderate effects, but a diversity increase and a slightly more significant increase of *Faecalibacterium* spp. were observed. These data indicate that Maillard products may have an unconventional prebiotic effect by the stimulation of *Faecalibacterium* and *Blautia* species.

Reference: Anton, P. M., Craus, A., Niquet-Leridon, C., and Tessier, F. J. (2012). Highly heated food rich in maillard reaction products limit an experimental colitis in mice. Food Funct, 3, 941

Poster 3

Synthesis and characterization of nickel oxide thin film and nanoparticles for hole transport in an all-inorganic colloidal quantum dot LED

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Nickel oxide thin film and nanoparticles are investigated for their application as a hole transport layer for all-inorganic quantum dot light emitting devices. The nickel oxide thin film is formed by annealing a spin coated layer of nickel hydroxide at 500 °C. The XRD, XPS and Raman measurements indicate that the formed nickel oxide thin film is non-stoichiometric with nickel vacancies. The ratio of Ni to O in the film, as calculated from the XPS measurement, is 1:1.7. The band gap of nickel oxide thin film calculated from the excitonic peak in the absorbance spectrum is 3.3 eV. The broad peak in the visible region of the absorbance and emission spectra indicate the presence of defect or trap states within the bandgap of the material. The overlap of the absorbance spectrum of quantum dots with the defect related emission spectrum of nickel oxide indicate that the thin film hole transport layer operates under energy transfer mechanism. Moreover, the quantum dot photoluminescence intensity is increased when in contact with the nickel oxide layer. This can be attributed to additional excitons created in the quantum dots as a result of energy transfer from the adjacent nickel oxide defect states. The schematic of the energy transfer mechanism and PL enhancement is depicted in the Fig. 1. Nickel oxide nanoparticles are synthesized by drying a solution of nickel hydroxide and annealing the dried powder at 360 °C. The obtained power is then dispersed in a polar solvent for further studies. In contrast to the thin film nickel oxide, the nanoparticles show signs of stoichiometry in the atomic ratio. The band gap the nanoparticles as calculated form the absorbance spectrum is 4.3 eV. Based on the band alignment to the quantum dot emissive layer, the nanoparticle hole transport layer operates under direct injection mechanism.

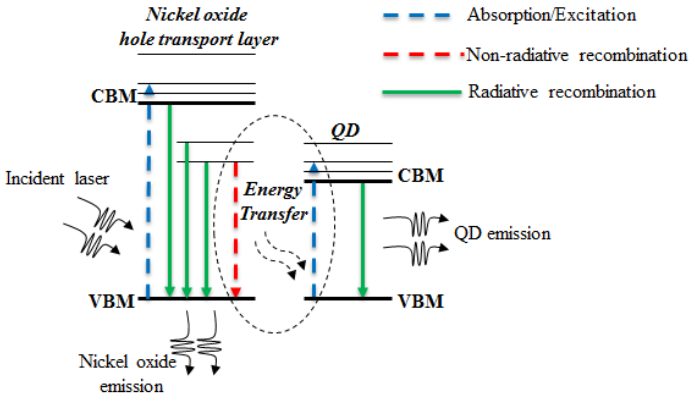

Fig. 1. Schematic representation of the energy transfer mechanism between the nickel oxide thin film and CdSe/ ZnS quantum dot.

Poster 4

Measuring functional implications of inhomogeneous Acetylcholine distribution in cerebral cortex

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Neuromodulators are critical for sensory information processing in cortical microcircuits. Acetylcholine (ACh) is a neuromodulator associated with attention, arousal, learning, and memory. Dysfunctional ACh modulation is associated with various neural disorders including Alzheimer's disease. Previous studies do not address the possibility that ACh concentrations are not spatially uniform. The effect of nonuniform ACh concentration gradients across the spatial extent of a microcircuit on the function of the microcircuit is not well understood yet. To better elucidate the effects of ACh on a neural circuit, we have combined an implanted microdialysis probe with a microelectrode array in anesthetized rat somatosensory cortex. Acetylcholine is administered via the microdialysis probe and the concomitant neural activity is recorded with the microelectrode array. Here we present preliminary results demonstrating that neural response to somatosensory (whisker) stimulation depends on the spatial gradient of ACh. Our initial results constitute the first steps towards better understanding the effect of inhomogeneous distribution of ACh on sensory information processing.

Poster 5

Revealing Bacterial Responses to Environmental Changes using Super-Resolution Microscopy

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Histone-like nucleoid structuring proteins (HNS) play significant roles in shaping the chromosomal DNA, regulation of transcriptional networks in microbes, as well as their responses upon environmental changes such as temperature fluctuations. In this study, we are studying the intracellular organization of HNS proteins in E. coli bacteria utilizing super-resolution microscopy, which surpasses conventional microscopy by 10-20 fold in resolution, and, more importantly, exploring the changes of of the spatial distribution of HNS proteins when the bacteria encounter various sudden environmental conditions, such as temperature fluctuations, drops in the pH values of the environment, and changes in ionic strengths of the bacterial growth medium. To quantify the spatial distribution of HNS in bacteria and its changes, we are implementing an automatic method based on Voronoi diagram. Localized HNS proteins from super-resolution microscopy are segmented, and clustered based on several quantitative parameters, such as areas, densities and mean distances of the k-th rank, computed from the Voronoi diagrams. These parameters, as well as the clustering analysis, allow us to quantify whether and how the spatial organization of HNS proteins responds to environmental fluctuations, and provide insight into understanding how microbes adapt to new environments.

Poster 6

Understanding electron energy loss mechanisms in EUV resists using photoemission and electron energy loss spectroscopies

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In order to continue to enhance the performance of computers, processes to efficiently and accurately manufacture nanoscale processors must be developed. One such process, Extreme Ultraviolet (EUV) Lithography, involves exposing photoactive resist materials to high-energy UV light, the resulting reaction changing the solubility of exposed areas to allow for chip patterning after development.[1] In this work, we have examined novel organometallic resist materials [2] (diphenyl tellurium diacrylate, triphenyl antimony diacrylate, tricyclohexyl antimony diacrylate, and triphenyl bismuth diacrylate) using X-ray and UV Photoemission Spectroscopies (XPS and UPS), and Electron Energy Loss Spectroscopy (EELS) to understand the key mechanisms by which excited low energy electrons (E < 90 eV) interact with, and deposit energy into resist films. Under ultra-high vacuum conditions, we explored the electronic structure of resist thin films using XPS and UPS aided with electronic structure calculations. Subsequently, we exposed the resist samples to electron beams of varying energies (E = 30, 50, 70, 90, 110 eV), measuring energy loss channels with EELS, while using XPS and UPS to monitor chemical changes in the films. Using empirical calculations to predict the chemical shift of core-level metal XPS peaks based on their coordination, we were able to propose a mechanism, consistent for all four resists, leading to the formation of stable di- or triphenyl metal compounds embedded in a new cross-linked polymer.

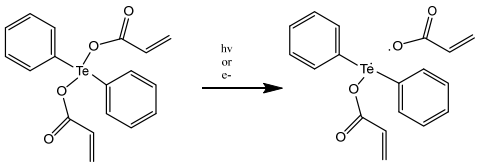

Fig.1. Initiation of the polymerization mechanism of diphenyl tellurium diacrylate proposed in this work.

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Poster 7

Measuring Nonlinear properties of Graphene Thin Films Using Z-Scan Technique

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The nonlinearity optics of two dimensional nanomaterials, specifically graphene, plays a significant role in various photonics devices since graphene is finding its usefulness in handling the enormous heat in nanoscale high density electronics. However, the experimental nonlinear study of graphene materials and then applying it to develop future optoelectronic devices needs more research.

The main goal of our research is to investigate the nonlinear properties, including nonlinear refractive index (n_2), nonlinear absorption coefficient (β), and thermo-optical linear and nonlinear coefficient (dn/dT), of graphene thin films by using a simple and sensitive technique, Z-scan, as shown in Fig. 1. In the Z-scan method, the sample is moved in the propagation direction (z) of a Gaussian beam that is narrowly focused. The transmitted signal of the materials, as a function position relative to the beam waist, is observed using a photodetector placed behind a small aperture.

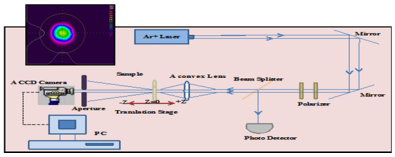

Fig. 1. Illustration of Z-Scan System Experimental Setup

In this research work, the Beta-Barium Borate (β-BaB2O4 or BBO) crystal has been chosen as an excellent candidate to calibrate the built Z-scan system and extract the thermal nonlinearity important to its remarkable properties. First, UV-vis spectroscopy, Raman spectroscopy, atomic force microscopy (AFM) and X-ray diffraction (XRD) are used to optically characterize the samples in the linear regime. The result for the BBO thermo-optical coefficient and nonlinear refraction were found to be $-2.2*-10^{-6}$ /^{0}C and $4.0056*10^{-11}$ cm^2/W. Moreover, the value of nonlinear absorption coefficient (β) for nonfunctionalized graphene thin film (NFG) is around $5.58*10^{-2}$ and $6.42*10^{-2}$ cm/W when deposited with gold nanorodes (AuNFG), concluding that gold nanorodes enhances the nonlinear properties of graphene materials. Thus, using nanostructures for the ability to control the thermal-optical behaviors not only increases but also opens the doors for new application areas, including biomolecular and chemical sensing, cooling systems, photo-thermal therapy, and photonics devices [1].

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Poster 8

Transport Properties of Cobalt Doped ZnO/p-Si Heterojunction Using Impedance Analysis and Exciton Lifetime Measurement

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In this study cobalt doped ZnO nanorods were grown on the boron doped p-type silicon wafers using chemical bath deposition method. Structural and electrical properties were examined using PL and impedance spectroscopy. XRD analysis revealed that all the doped ZnO nanorods were in hexagonal wurtzite structure and demonstrated good crystallinity and a preferable *c* axial orientation. We observed an increase in intensity along (002) direction with increase in cobalt concentration. Moreover, transport properties of ZnO/p-Si heterojunctions were investigated using ac impedance spectroscopy in the frequency range of 10 Hz to 20 MHz with and without biasing. As the doping is varied, the resistance decreases rapidly with doping. In addition, we performed impedance measurements on ZnO/p-Si heterojunctions under different annealing temperature (100 ^{0}C to 400 ^{0}C) and transport properties of the samples were investigated by measuring the real and imaginary parts of the impedance function. We have proposed a resistance-capacitance (RC) model to explain electrical impedance properties of the ZnO/p-Si heterojunctions. In addition, ZnO nanorods were examined using time resolved photoluminescence measurement which provides the information about exciton lifetime. We will discuss the variation of an exciton lifetime with different cobalt doped samples.

Poster 9

Direct Two-photon Absorption Induced Emission of InAs/GaAs Quantum dots

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Semiconductor quantum dots (QD) provide 3-dimensional confinement of carriers. The resulting atomic-like energy levels, size-dependent electrical and optical properties, as well as broad range of technological applications have made QDs widely studied during the past three decades. Self-assembled III-V QDs which form on a wetting layer (WL) are the most studied semiconductor QDs because of their well-established fabrication techniques and versatile optical properties. As one of the most interesting non-linear optical properties, two-photon absorption (TPA) in In(Ga,Al)As QDs has been used for both fundamental physics studies and engineering applications such as Rabi oscillation[1], up-conversion luminescence[2], inter-band solar cells[3]–[5] and infrared photodetectors[6]. All previous research has been through two-photon excitation with energy either higher than the matrix bandgap or within the sub-band of the QDs. Whereas investigating of direct TPA in the QDs has not been reported.

We present a photoluminescence (PL) study of undoped InAs/GaAs QDs induced by direct TPA with excitation near the QD half-bandgap. A gradient density QD sample grown by molecular beam epitaxy (MBE) is used in this study to compare QD effects with those of the WL only. Power dependent PL using both above bandgap cw excitation, and below bandgap (half the QD ground state energy) pulsed excitation are well fit by power laws of approximately integer order[7]: two-photon processes are indicated by higher order power laws of the same system under pulsed excitation. Two-photon photoluminescence excitation (TP-PLE) further provides evidence of direct TPA into the QDs and the WL when the two-photon excitation energy is resonant with the QDs states and the WL states. The implications of the varying power laws will be discussed.

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Poster 10

Investigation the conditions of the conformal shell layers formed by different types of PVD techniques on different aspect ratio nanorods arrays.

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Manufacturing of batteries, solar cells, sensors and fuel cells have been greatly depended on core/shell nanorods arrays and their coated forms due to the defect-free interface concerns, fabrication of the conformal shell layers on nanorod arrays has been a great challenge. Monte Carlo (MC) simulations to estimate the most favorable deposition condition to produce a conformal shell coating. For this reason, MC methods became a favored simulation technique for physical vapor deposition. We studied different height effects of the arrays on the conformality of the coating. Our results indicate that conventional PVD techniques, which offer low cost and large scale thin film fabrication, can be utilized for highly conformal and uniform shell coating formation in device applications.

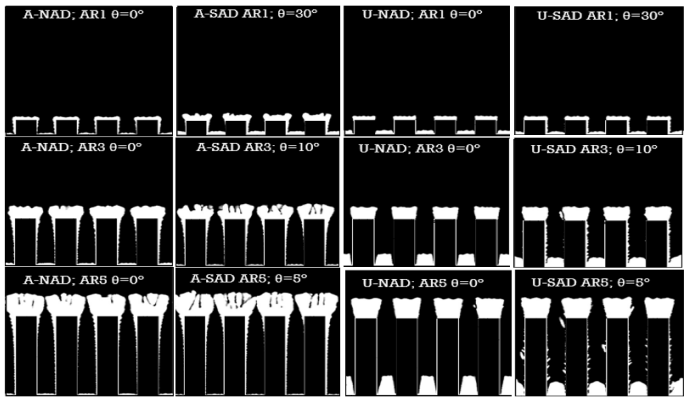

Fig. 1. A snapshot for MC simulation results for nanorod arrays coated with different flux types. Small angle depositions were also performed at different deposition angles of $\theta = 30^{o}$, 10^{o}, and 5^{o}, which were chosen for each different aspect ratio value.

Poster 11

Dual-width plasmonic gratings with tunable optical enhancement for Raman spectroscopy substrates

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Plasmonic gratings have been demonstrated as effective for producing optical enhancements upon incident light irradiation in different applications.[1], [2] Making use of a previously developed nanomasking technique for fabricating sub-10 nm gaps between plasmonically active structures, gratings with two repeated widths per period have been demonstrated.[3], [4] The two grating structure widths are separately controllable, allowing for the design of desirable combinations for optimal enhancement at specific incident wavelengths. Computational electromagnetic simulations of dual-width gratings demonstrate that the ability to controllably tune the widths separately from one another is important for optimally producing enhancement at different wavelengths.[5] Sweeping of the structure widths and heights, gap width, period, and incident wavelengths demonstrate that it is necessary to optimize all of the geometrical parameters simultaneously in order to obtain the peak enhancement. A custom Raman spectroscopy setup is used to characterize the usefulness of fabricated structures as surface-enhanced Raman substrates.

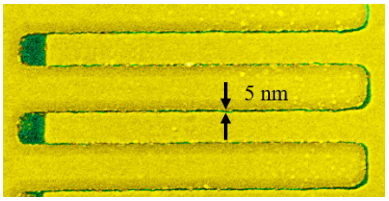

Fig. 1. Colorized SEM image of a dual-width grating

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Poster 12

Digitization and Additive Manufacturing of Natural Surfaces

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Natural surfaces have been a great source of inspiration for producing surfaces with a wide variety of functionalities and applications. Different techniques have been utilized for producing bioinspired surfaces such as soft lithography [1], ion beam roughening [2], and nanocasting [3]. With the advent of CAD/CAM systems, digital models combined with 3D printing techniques have shown to be very promising routes for surface fabrication. Using high resolution 3D laser scanning microscopy, it is possible to digitize the surfaces of interest such as surfaces found in nature with less than 200 nm resolution. Using advanced additive manufacturing techniques, such as direct laser writing, the digitized surfaces with micro and nanoscale features can then be fabricated. Here we show the proof of concept of scanning a surface found in nature using a 3D laser scanning microscope, obtaining the CAD model of the surface and printing it using a 3D laser lithography system.

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Poster 13

Photoluminescence study of InN/GaN multi-quantum well under biaxial strain

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A low temperature photoluminescence (PL) study was conducted on InN/GaN multi-quantum well structures that are grown by molecular beam epitaxy. A decline of quantum well emission intensity was observed as the sample temperature was increased. This decline is most likely caused by exciton separation and the binding energy can be determined by the function of PL intensity versus temperature. A red shift of GaN barrier emission was observed when InN thickness exceeded 3ML. This shift is possibly caused by a strain change at each InN/GaN interface, which implies that a critical thickness of InN was crossed.

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Poster 14

ELECTROCHEMICAL-STM INVESTIGATION OF SILVER HALIDE MONOLAYERS ON A AU(111) SURFACE

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In previous research completed by Iski et al.[1], it was found that through specific electrochemical methods, a silver (Ag) monolayer could be formed on a Au(111) surface in both a chloride-free and chloride-rich solution. The electrochemical method used was under potential deposition (UPD). The previous study showed that, in a chloride-free environment, the Ag monolayer could be formed and atomically resolved; however, once removed from the cell, it could be completely destroyed via hydrogen flame annealing. Interestingly, in the presence of chloride, the same Ag monolayer was formed and was found to be extremely thermally stable after removal from the cell and was resistive to temperatures as high as 1,000 K. The atomic structure of these films can be studied with electrochemical scanning tunneling microscopy (EC-STM), which not only allows for atomic scale imaging of the surface layer within an electrochemical environment, but also facilitates the taking of cyclic voltammograms (CVs), which can be used to examine the redox behavior of the systems. Despite many studies on these types of surface layers[2], very few publications have directly studied their extreme thermal stability. Since it is known that the stability of bulk metal halide structures decreases as the halogen ion increases in size, an investigative study was performed following the same procedure, substituting chloride with bromide. As with the $AgCl_x$ system, once $AgBr_x$ was used to form the Ag monolayer, a new surface structure formed which was also thermally resistive to a hydrogen flame. CVs taken in the same region as those of the previous work show a definite surface modification by $AgBr_x$. Further electrochemical studies into these Ag monolayers formed in a halogenated environment are being conducted in an attempt to better understand the properties of these surfaces and the type of redox chemistry occurring at the relevant potentials. Furthermore, density functional theory (DFT) will also be used to look at the equilibrium coverage and the diffusion barrier of the bromide on the Ag monolayer. Using EC-STM and DFT, we plan to study the ways in which this remarkable stability is imparted to the single crystal surface under ambient conditions.

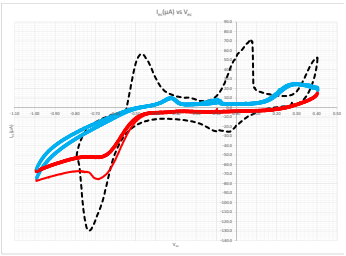

Fig. 1. Overlap of CVs for AgCl (solid lines) and AgBr (dotted black) taken after UPD of Ag was performed.

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Poster 15

Surface Texturing for Friction Reduction via 3D Printing

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The introduction of surface-texturing is one of the most effective ways to enhance the tribological performance of interfaces because it reduces the real contact area and consequently, the friction forces between the surfaces. Current manufacturing methods, such as laser surface-texturing and photolithography, allow the fabrication of regularly shaped protrusions and holes, which induce precise functionalities to the engineered surface. Although powerful, those techniques are limited to patterned structures with the same height. Furthermore, pricey and laborious pre- and post-processing steps are required. Additive manufacturing is an alternative to create surface textures with more design flexibility and little or no need for pre- or post-processing. Herein we demonstrate the applicability of a desktop 3D printer in the fabrication of surface textures for investigation of their effects on the friction forces and wear resistance.

A fused deposition modeling 3D printer was used to make polylactic acid samples from files modeled in Solidworks. Surface texturing was introduced by designing hollow cylinders on sample surfaces, which were arranged in different density with uniform or random-height. Graphite was applied by spray coating on a group of samples to investigate chemistry modification of textured surfaces. Linear reciprocating friction test was performed to evaluate the different types of surfaces. Results show that the addition of graphite significantly reduced the coefficient of friction (COF) by 50%. The lowest COF results were from the uniform height textures, which may be explained by a better load distribution among the cylinders during friction test. Furthermore, the graphite on the uniform height textures was worn off more evenly than that on the textures with random height.

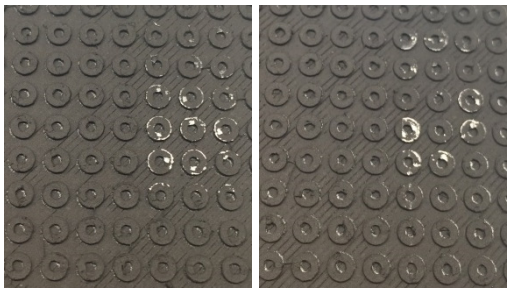

Fig. 1. Uniform height textures on left-hand side and random height texture on right. It is noticeable that the graphite was removed more intensively on some of the cylinders of the random textures.

Poster 16

The nature of metal-insulator transition in ultrathin $SrVO_3$ films*

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Paramagnetic metallic oxide $SrVO_3$ (SVO) is an itinerant system known to undergo thickness-induced metal-insulator transition (MIT) in ultrathin film form, which makes it a prototype system for the study of the mechanism behind metal-insulator-transition like structure distortion, electron correlations and disorder-induced localization. We have grown $SrVO_3$ thin films with different thicknesses with atomically flat surface through the layer-by-layer deposition by laser Molecular Beam Epitaxy (laser-MBE) on $SrTiO_3$ (001) (STO) surface. Ultraviolet Photoemission Spectroscopy (UPS) measurements confirm a metal-nonmetal crossover at the thickness of ~3 unit cell as reported before [1], while Low Energy Electron Diffraction (LEED) measurements reveal that there is a corresponding evolution of surface structure to $(\sqrt{2}\times\sqrt{2})R45^\circ$ reconstruction for films with thickness of above 3 unit cell. Atomically resolved Scanning Transmission Electron Microscopy (STEM) and Electron Energy Loss Spectroscopy (EELS) analysis show depletion of Sr, change of V valence and the existence of a significant amount of oxygen vacancies in the first three unit cell above the interface, thus providing a likely driving force of the metal-nonmetal transition.

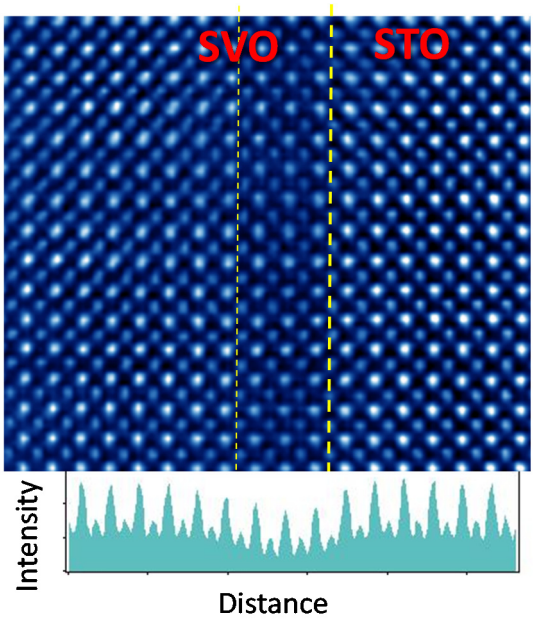

Fig. 1. Z-contrast STEM image and intensity profile along [100] direction, showing a distinct difference between the first 3 unit cell and the rest of the SVO film.

*This work is supported by U.S. DOE under Grant No. DOE DE-SC0002136. GW was partially supported by the National Science Foundation under the NSF EPSCoR Cooperative Agreement No. EPS-1003897 with additional support from the Louisiana Board of Regents.

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Poster 17

Engineered Surfaces with Deformation-Resistant Core-Shell Nanostructures

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Surface nano-texturing is an attractive method for designing surfaces with improved tribological properties, particularly for micro/nano-electro-mechanical systems (MEMS/NEMS) applications. However, a common weakness of nano-textured surfaces is a lack of structural integrity when subjected to contact loading, resulting in permanent deformation of the engineered surface at even moderate contact forces encountered in microscale systems. To address this issue, patterned engineered surfaces comprised of arrays of novel Al/a-Si core-shell nanostructures (CSNs) with high durability and ultra-low friction have been developed. When subjected to nanoscratch testing using a diamond tip, these surfaces are shown to have extremely low coefficients of friction (~0.06), as well as no detectable nanostructure deformation at contact pressures in excess of 1 GPa. Further nanomechanical characterization on individual CSNs reveal that this deformation resistance is due to an unconventional mechanical response, as shown in Fig. 1(a), that is enabled by dislocation activities within the confined Al core. Specifically, it is hypothesized that dislocations nucleated within the Al core during loading retrace their paths and annihilate after the applied load is removed, leading to recovery of plastic deformation. This is supported by molecular dynamics simulations that show the dislocation content generated at the maximum indenter displacement (full load) is substantially reduced after the applied load is removed (full unload), and eventually becomes free of dislocations at equilibrium, as seen in Fig. 1(b). The unique mechanical properties of these CSNs provide avenues for designing engineered surfaces that could benefit a variety of fields, including MEMS/NEMS, microelectronics, magnetic recording, or any other application when the mechanical integrity of nanostructures is important.

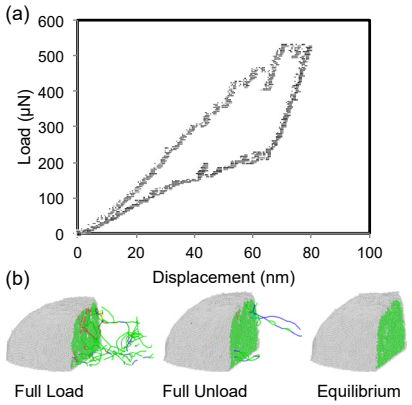

Fig. 1: (a) Load-displacement plot for an 80 nm indent on a CSN, showing no residual deformation after loading; (b) snapshots of dislocation content within the core of a CSN.

Poster 18

$SrRuO_3$ (111) thin films with persistent $(\sqrt{3} \times \sqrt{3})R30°$ surface reconstruction*

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Abstract

The six-fold symmetry provided by the (111) surface of simple cubic perovskite oxides allows the epitaxial growth of novel quantum materials with honeycomb lattice structure such as topological insulators. However, the strong surface polarity posts an extreme challenge of stabilizing grown materials along such a polar [111] direction. It is known that $SrRuO_3$ (SRO), an itinerant ferromagnetic system, exhibits enhanced instability but also enhanced magnetism as thin film from grown along [111] compared with [001] direction, while the origin is unclear. We have studied high quality SRO films grown on $SrTiO_3$ (STO) (111) with laser-MBE, low energy electron diffraction, and angle-resolved X-ray photoelectron spectroscopy (ARXPS). With Ti-terminated STO (111) substrate, SRO films are grown with layer-by-layer fashion confirmed by reflection high energy electron diffraction (RHEED). However, the surface exhibits a $(\sqrt{3}\times\sqrt{3})R30°$ reconstruction with respect to a cubic-like structure inside the films, regardless of the film thickness. Such reconstruction cannot be simply understood with the results of orthorhombic structure existing in the bulk of SRO. ARXPS results indicate that the reconstructed $SrO_{3-\delta}$ surface is off-stoichiometric from bulk-truncated SrO_3 layer with an estimated value of $\delta \sim 0.5$. The reconstruction likely originates from the reduction of surface. In addition, the films with thickness below 4 u.c. are nonmetallic and non-magnetic, in contrast to the bulk material.

*This work was supported by US DOE DE-SC0002136. Weimei Xie was supported by China Scholarship Council.

Poster 19

Surface structural phase transition of IrTe2 studied by LEED

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Here we report on the temperature dependence and reversibility of the surface structure observed by LEED for single crystals of of $IrTe_2$. $IrTe_2$ contains stacked layers of hexagonal Ir lattices sandwiched between Te layers with octahedral coordination. In the bulk there are two structural transitions happened at 280K and 180K during cooling process, but only one transition at 280K during heating process [1]. There is hysteresis in resistivity and a sharp peak in specific heat around 280K [2], indicating a first-order phase transition in the bulk. However, the surface measurements imply different nature of the structural transition. The IrTe2 samples used here were cleaved *in situ* at 300K, exposing Te layer, For cooling cycle, the fresh cleaved surface shows 1x1 bulk truncated pattern at 300K, as it is cooled it reconstructs into a 1x5 , when the sample is cooled down further a 1x8 pattern emerges, which is not completely stable, and finally a 1x6 LEED pattern is observed at lowest temperature, i.e. the ground state. Detailed analysis of the 1x8 diffraction pattern suggests this surface has broken reflection or inversion symmetry. For heating cycle, the surface follows a different path: it stays at 1x6 pattern up to higher than 200K, until a 1x8 pattern emerges. Around 288K, there is weak 1x5 like feature with much larger fractional spot line width compared to integer ones. This indicates a crossover of phase transition with structural instability from the 1x8 to the 1x1 phase. Such 1x5 feature is not observed in the bulk during heating process, indicating the intrinsic properties of the surface structural transition is much different than the bulk. Further observations show coexistence of multiplephases at various temperatures and length scales. The overall features resemble the “devil’s staircase” phenomena under the competition of commensurate and incommensurate orders.

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Poster 20

Bias-dependent rotation of thiol-tethered molecules on Au(111)

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Using azobenzene with alkane-thiol “tethers” (ABT) to Au(111), molecular rotation is induced by lowering potential barriers to motion, instead of the more common method of imparting kinetic energy to the molecule to hop into a so-called active site[1]. On the reconstructed Au(111) surface, ABT decorates the elbows of the herringbone reconstruction at low coverage (Fig1a). Despite the seeming similarity in adsorption sites, topographic images of the molecules recorded at 80 K vary from linear, to "multi-tined," to “disk,” due to thermally driven reorientation. In effect, the images capture dynamical states. From this variation in orientational images, we may deduce the thermally accessible landscape of the local potential energy surface. Remarkably, upon lowering the sample bias to near-zero, we observe that flat, stationary molecules appear as concentric rings. The rings can be readily assigned to the circles traced by the two benzenes of the headgroup as they stand on-edge and rotate while tethered to the Au-S anchor. The observed motion lends itself to the description of "hovering and twirling". The motion can be understood to be induced by the van der Waals attraction of the molecule to the approaching tip. The picture is rationalized by adapting existing physisorption potentials of benzene [2] and modeling Ag tip and Au substrate as two approaching surfaces with separation controlled by the junction bias. The model reproduces the observations, as illustrated in Figure 1. At separations d > 11 Å between the surfaces, the azobenzene head group lies flat; at a junction gap of 9 Å, the hovering potential develops in which the on-edge, simultaneous adsorption of the molecule to the tip and substrate becomes the global minimum. The images of motion elucidate dynamics driven by van der Waals forces.

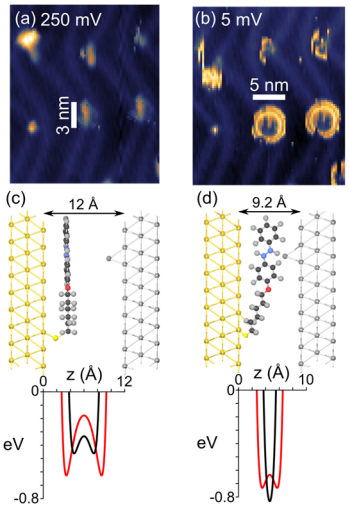

Fig. 1. (a) At V_B = 250 mV, ABT is stationary and lies flat on Au(111), (b) at V_B = 5 mV, ABT twirls with benzenes of the headgroup standing on edge. (c,d) The observations are rationalized by the physisorption potentials given in Morse form for flat (red) and on-edge (black) adsorption potential on the approaching tip and substrate.

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Poster 21

Real-Space Analysis of Scanning Tunneling Microscope Images: Accurate measurements of local structure and disorder

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Scanning tunneling microscope (STM) images of ordered surfaces can cover hundreds of unit cells with good resolution of each atomic or molecular feature. We index these image features and study their positon compared to the other symmetry equivalent features and the best-fit lattice. Using software we have developed in Matlab, we have analyzed STM images of graphite(0001) and alkanethiol self-assembled monolayers (SAMs) on Au(111). The features are identified and located by a cross-correlation of the image with a 2D Gaussian kernel. We determine the local distortion from the feature locations by using known symmetry of the crystalline surface (from e.g. x-ray diffraction) as an internal standard[1]. We then modify the locations of these features using models of distortion due to piezoelectric hysteresis, piezoelectric creep and sample drift[2]. By using the locations of these indexed features on alkanethiol SAMs, we have made measurements of decanethiol chain tilt direction and angle by measuring longer-chain thiols mixed within the SAM; as well as deviations of each basis feature location from the best-fit lattice as a measure of conformational flexibility. Similar measurements on graphite have highly localized image features, giving some insight on the fundamental position resolution of the STM. In the future, we plan to analyze other measurements that could be associated with individual surface features using this technique, including defect density and structure variation around defects and boundaries.

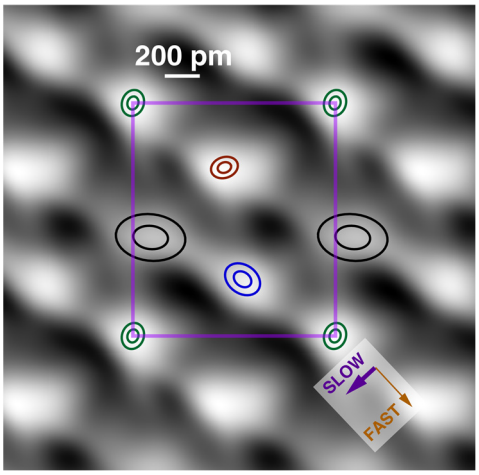

Fig. 1. *A lattice averaged STM image of 1361 unit cells from an STM image of a C10 SAM. The rectangle shows the (2√3×3)rect. unit cell. The one and two sigma probability ellipsoids are shown for each of the 4 basis molecules. The fast and slow scan directions are also shown.*

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Poster 22

Local Dynamics and Disorder of the Terminal Methyl Groups in *n*-Alkanethiol Self-Assembled Monolayers on Au(111): A molecular dynamics study

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In our present work, molecular dynamics has been used to study the configuration of the chain termini of *n*-alkanethiol SAMs in comparison with the corresponding STM images of SAM-air interface. Although the position of both the methylene backbone and the terminal methyl groups are highly restricted by the SAM lattice, we experimentally observe an apparent anisotropic probability distribution of the chain termini within their respective lattice sites. In order to gain physical insight into the possible origins of this anisotropy, we have undertaken a study of the local dynamics and disorder at the SAM surface using molecular dynamics simulations. For our model of the SAM surface, a systematic study has been carried out with different forcefields and initial configurations. We have used the canonical ensemble during the relaxation process and microcanonical ensemble for the subsequent dynamical analysis. We fix the sulfur atoms to the $(\sqrt{3} \times \sqrt{3})R30°$ lattice sites of Au(111) and focus our analysis on the dynamics and disorder of the alkyl chain termini, quantified using the statistics of the methyl group trajectory, orientation of the terminal C–C bond, chain twist angle, gauche fraction, an radial distribution function. Control of the SAM structure is achieved in our model through definition of the orientation of the S–C bond as a proxy for the poorly understood details of the Au surface reconstruction and the S adsorption sites. Our studies confirm the influence of the geometry of the Au-thiol interface on the dynamics of the terminal group.[1,2] Along with the dynamics of the terminal group, we have also studied the tilt and twist angle of the backbone, density profile along the surface normal, and the rotational dynamics. The simplicity of the current system allows us to extend the calculation over different terminal groups, different substrates and system with mixture of different alkanethiol molecules.

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Poster 23

Exploring Macro Porous Silicon as a Substrate for Heterojunction Solar Cells

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In this study, we explore the interfacial electronic properties of macro porous silicon (PoSi) with the goal of producing an electronically-perfect high-surface-area silicon substrate. Photoelectrochemical etching of n-type Si(100) in aqueous HF is performed with back-side illumination. We use a novel dual feedback approach for etching that allows simultaneous control of both the cell voltage and cell current. The as-produced PoSi exhibits photoluminescence due to electronic surface defects, quantum confinement, and the nanostructures formed on the surface before the macro pores nucleate. We have explored combinations of polishing and thermal oxidation to systematically remove the pre-pore nucleation nanostructure and the photo luminescent surface defects, respectively. Electrical characterization of PoSi-Pd Schottky diodes show that these treatments greatly reduce the electronic defects. Coating the macro pores with colloidal quantum dots (CQDs) forms a high surface area p-n heterojunction which has the potential to simultaneously increase the optical path length for absorption by the quantum dots without significantly increasing thickness of the CQD film with respect to carrier transport and extraction. Preliminary experiments using PbS CQDs will be discussed.

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Poster 24

Electronic states and optical transitions in the semiconductor layered biconical quantum dot

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The electronic states in the *GaAs* layered biconical (superellipsoidal) quantum dot (QD) in a strong and weak size quantization regimes are theoretically investigated within the framework of the geometrical adiabatic approximation. The effect of the jump discontinuity of the step-like potential at the surface of the QD and the coating layer on the electron localization around the geometrical center of the QD is revealed. An atypical linear term in the effective confining potential forms a family of non-equidistant sublevels in the electron energy spectrum due to the QD shape. In the weak size quantization regime the motion of the exciton's center-of-gravity is quantized, which leads to the appearance of the additional Coulomb sub-levels in the energy spectrum of the QD. The direct interband absorption of light in the layered biconical QD is also considered in both strong and weak size quantization regimes. The dependences of the absorption edge on QD geometrical parameters are revealed. Corresponding selection rules for quantum transitions are obtained as well.

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Poster 25

Vertical electrical field induced monolayer island growth on $TiSe_2$

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Emerging 2D materials, such as atomically thin transition metal dichalcogenides (TMDCs), have been the subject of intense research efforts due to their fascinating properties and potential applications in future electronic and optical devices. The interfaces in these 2D materials, including domain boundaries and edges, strongly govern the electronic and magnetic behavior and can also potentially host new quantum states [1]. On the other hand, these interfaces are more susceptible to thermal fluctuation and external stimuli.

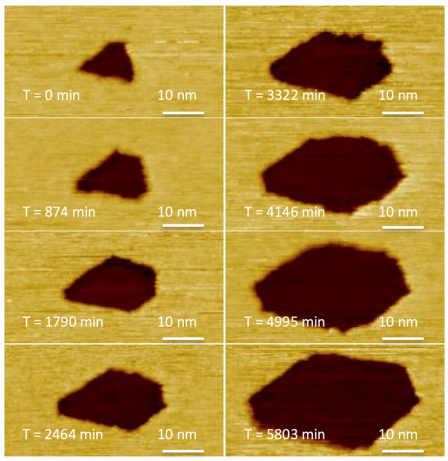

Fig. 1. Vertical electrical field induced monolayer vacancy island growth on

For practical applications of mono- and few-layer TMDCs, it is essential to characterize the structural stability under external stimuli such as electrical fields. Using monolayer vacancy islands on titanium diselenide ($TiSe_2$) surfaces as a model system, we experimentally and theoretically investigated the shape evolution and growth rate by using scanning tunneling microscopy (STM). The growth rate depending on the tunneling current is experimentally determined. Our simulations of shape evolution that use a phase-field model are well consistent with the experimental observations. The results from this study could be potentially important for electronic applications of atomically thin TMDCs and other 2D materials.

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Poster 26

Ordering of Organics on (111) Coinage Metals: Substrates Matter

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On Cu(111) anthraquinone (AQ) forms a dramatic giant honeycomb lattice, with pores over 5 nm across [1]. While many honeycomb lattices of organic molecules have been reported, this one is especially remarkable because of its regularity and because the sides of the honeycomb are longer than one molecular constituent (in this case, 3). After attempts to account for the pore size in terms of Friedel oscillations of the well-known metallic surface state of (111) coinage metals, an alternative proposal invoked a picture of closed-shell 2D pseudoatom/quantum dots [2], including shifts to the surface state due to a perpendicular electric field from charge transfer at the surface [3]. To test this picture, we investigated AQ adsorbed on Au(111) [5], for which the surface state has a different Fermi wavelength and mass (and a lattice constant that is 13% larger). DFT (VASP) provides guidance on key energies [3,4]. The ordered structure indeed is decidedly different, with no giant honeycomb but instead a small structure consisting of isolated 6-AQ pinwheels. Other structures are seen at different AQ coverages. In particular, higher AQ coverages exhibit disordered close-packed islands with linking chains. The distribution of pore areas is lognormal distribution, rather than gamma or generalized Wigner [GWD] often found for surface structures [6]; the underlying physics likely is that random noise is involved in their formation. Similar occurrences of log-normal distributions in other contexts are discussed.

Work supported in part by NSF Grant No. CHE 13-05892.

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Poster 27

Electronic States and the Size-Quantized Stark Effect in the Semiconductor Semi-Ellipsoidal Quantum Dot

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The electronic states in a strongly elongated semi-ellipsoidal quantum dot (QD) of *GaAs* are theoretically investigated within the framework of the geometrical adiabatic approximation. The presence of an atypical linear term in the effective confining potential of the "slow" subsystem is revealed as a consequence of the specifically truncated QD's symmetry. For the lower levels of the electron spectrum, the localization of the electron in the vicinity of the QD geometric center of gravity, due to the influence of the QD surface curvature, is proved. The effects of the linear term of the effective confining potential and the competing term of the electrical field on the motion of the electron are considered. Both pseudo and quantum-confined Stark effects are considered. The possibility of implementation of an electron quasi-continuous spectrum over the lower energy levels of the "fast" subsystem is revealed.

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Poster 28

Surface Transport Study of Doped Ultra-Thin Sb Quantum Wells

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A topoelectronic transition is predicted for an Sb quantum well (QW) as a function of QW thickness [1]. Bulk Sb is a semimetal with a negative bandgap, with neither the conduction band minimum nor the valence band maximum at the Γ point. The Dirac point for the topological surface states is at the Γ point. Our goal is to study the transport properties of the topological surface states by suppressing the bulk conductivity through quantum confinement and enhancing the surface conductivity through remote n-type doping at the Γ point. Conductivity measurements on undoped QWs (0.7 to 6 nm thick) show a suppression of the bulk states, such that the surface conductivity is ~20% of the total conductivity for a 3.8 nm-thick QW [2]. Interpretation of Hall-effect measurements, which nominally indicate p-type conduction for undoped QWs, are complicated by the presence of both electrons and holes. We have begun experiments to populate the topological electron states by doping the GaSb barrier with Te atoms, creating donor states at the Γ point. At the Γ point of the QW, the topological electron states have a lower energy than any of the bulk conduction band minima. From Hall measurements at low magnetic field (<0.2 T), we observed that the apparent electron density decreases with decreasing GaSb spacer thickness (distance between the doped GaSb layer and the Sb QW) from 90 nm to 20 nm, as shown in Figure 1. This indicates that electrons are transferred from the doped layer to the Sb QW. Further measurements were performed at the National High Magnetic Field Laboratory with magnetic field up to 18T at a temperature of <50 mK. Carrier densities calculated using the Hall slope and the Shubnikov-de Haas oscillations were different from each other. Also, the Hall slope decreased with increasing magnetic field, indicating the contribution of multiple carrier channels. We are carrying out further analysis to separate the multiple carrier channels and determine the individual carrier densities and mobilities.

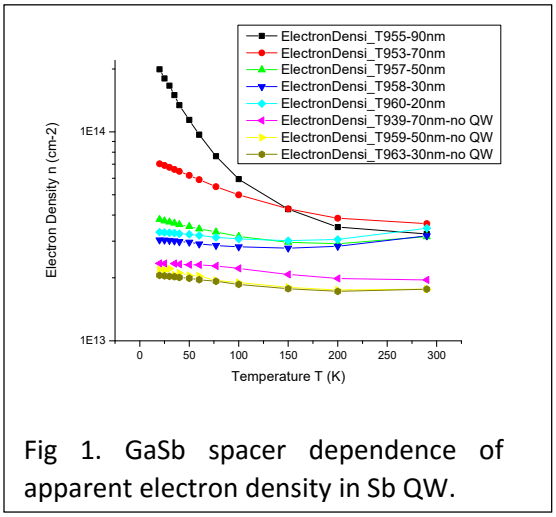

Fig 1. GaSb spacer dependence of apparent electron density in Sb QW.

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Poster 29

First Principles Calculations of Charge Density Waves in 2H-$TaSe_2$: Dependence on Layer Number and Temperature

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Tantalum diselenide ($TaSe_2$), a layered transition-metal dichalcogenide (TMD), is an electronically interesting material because it exhibits several phase transitions due to a delicate balance among competing electronic ground states. With decreasing temperature, the metallic ground state changes to an incommensurate charge density wave (ICDW) state at ≈ 122 K followed by a commensurate charge density wave (CCDW) state at ≈ 90 K, and eventually a superconducting state if the temperature decreases to ≈ 0.14 K. Questions remain on how changing the layer number of 2H-$TaSe_2$ could affect these transition temperatures. Using first principles calculations, we present the structural energetics, band dispersion near the Fermi level, and phonon modes at the Brillouin zone center for two specific variables: electronic temperature and layer number. Specifically, we calculate that the CCDW phase remains robust as the crystal is thinned down, even to single layer, and the transition temperatures increase. Our prediction finds new, low frequency Raman modes in the CDW states, which we also have observed experimentally in bulk samples. (Fig. 1 (a)). Theoretically, the E mode redshifts with increasing layer number while the A_1 mode blue shifts due to an enhancement of the effective electron-phonon coupling constant (Fig 1(b)). We also predict the electronic band structure and density of states (DOSs) at the Fermi level change as a function of reduced layer number. Our results open new opportunities to control the collective phases of TMDs and expand the tunability of key properties of 2D-materials for electronic applications.

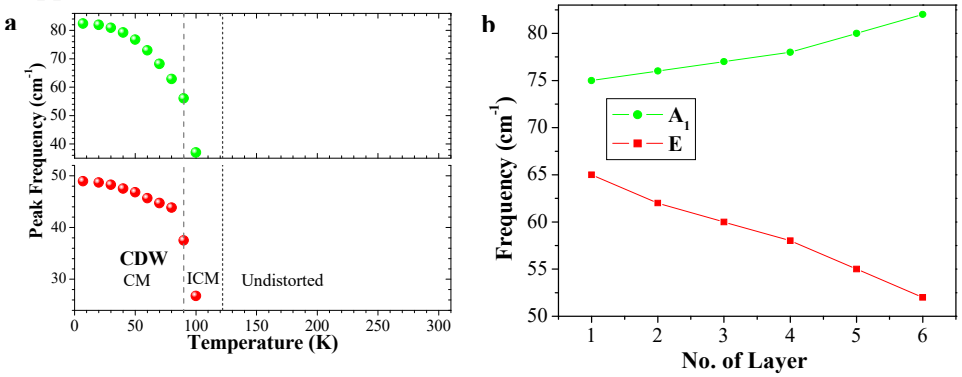

Fig 1: Low-frequency Raman phonon modes, which are nonexistent in the metallic state, arise in both the CDW states and depend sensitively on temperature and layer number. (a) Experimental observation of the peak frequency of the E and A_1 Raman modes as a function of temperature. (b) DFT predictions of the peak frequency of the E and A_1 modes as a function of layer number.

Session 4 notes:

Sensing the binding sites of RNAP Holoenzyme on λ phage DNA attached to a probe tip with Solid State Nanopores

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This study explores the detection of RNAP Holoenzyme specific binding sites on λ DNA molecules with an apparatus that integrates a Solid State Nanopore (SSN) with a Tuning Fork based Force sensing Probe tip (SSN-TFFSP). Using this apparatus, we can control the DNA translocation rate to be slower than >100μs/base or <1nm/ms in silicon nitride nanopores, a rate that is 1000 times slower than free DNA translocation through solid state nanopores[1]. This slow DNA translocation rate could provide sufficient temporal resolution to determine the individual RNAP binding sites on a λ DNA molecule. λ DNA has two promoter and three pseudo promoter sites for RNAP Holoenzyme to bind [2]. Schematic diagram for experimental set up is shown in Fig. 1. We show the results of free and controlled translocation of λ DNA with and without bound RNAP through solid state nanopores. To prevent the separation of RNAP proteins from a λ DNA molecule in the high electric field inside a nanopore, we covalently bound the RNAP Holoenzyme to the λ DNA by formaldehyde crosslinking. In order to bind DNA molecules to the streptavidin coated tip, a biotinylated primer was ligated to the one end of λ DNA molecules. We estimate the binding probability of the RNAP at various positions on λ DNA from free translocation data. The accuracy of determining the binding sites of RNAP with controlled rate translocation, will also be estimated and discussed.

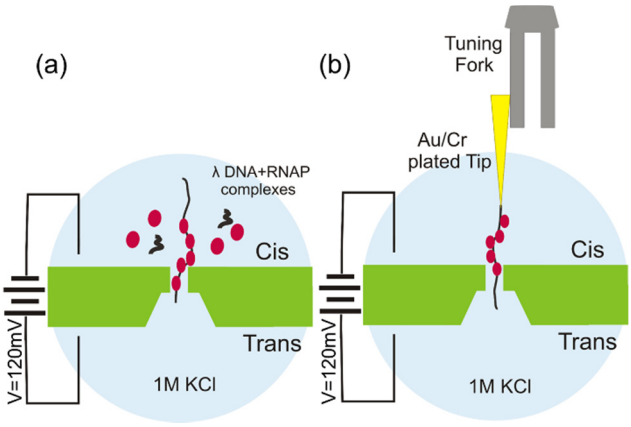

Figure1. (a) A schematic drawing of our experimental setup for free DNA translocation experiment. (b) A schematic diagram of our experimental setup for controlled translocation with λ DNA +RNAP complexes tethered to a probe tip

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Atomically Precise Design, Synthesis, and Characterization of 2D Material Interfaces

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Graphene continues to demonstrate exceptional electronic, optical, mechanical, and thermal properties, recently aided by developments in van der Waals heterostructures enabling strongly enhanced interfacial homogeneity. While these heterogeneous solids continue to uncover novel properties and applications for 2D materials, they are significantly limited to naturally occurring, air-stable, layered solids. Understanding and developing 2D interfaces beyond nature's limitations enables the realization of distinct *classes* of interface with novel properties, potential applications, and unique tunability. In this work, we discuss the formation of such novel 2D material interfaces and our efforts to understand them, particularly at the atomic scale. Initial work focused on unique synthesis required to achieve graphene on crystalline, noble metal surfaces, demonstrating the significance of the non-interacting surface for growth and studies of nearly intrinsic electronic properties in the 2D materials[1]. Following the initial work, this synthetic motif played a key role in the expansion of 2D crystals beyond air-stable, van der Waals solids[2,3]. The same inert crystalline platform subsequently enabled the development of 2D-2D interfaces at the surface of the metal; scanning tunneling micropscopy characterization clearly resolves unmodified, atomically pristine graphene-semiconductor van der Waals interfaces in both lateral and vertical configurations[4]. Finally, similar graphene-semiconductor interfaces are examined at the atomic scale to understand the highly anisotropic, covalent interface and its potential role in wafer-scale electomechanical manipulation[5].

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Xe Irradiation of Graphene on Ir(111): From Trapping to Blistering

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In this study we investigate the phenomena that occur during Xe ion irradiation of graphene epitaxially grown on Ir(111) by combining X-ray photoelectron spectroscopy, scanning tunneling microscopy, molecular dynamics simulations, and density functional theory calculations. Under conditions where without graphene nearly all ions are backscattered, with a monolayer graphene, these ions are trapped at the interface.

The graphene mesh acts as a one-way valve which upon annealing seals the trapped species in highly pressurized blisters (compare Fig. 1). We find that the one-way valve effect results from the fact that the energetic particles can easily penetrate the graphene, then lose most of their energy to the substrate, making a return through the covering graphene virtually impossible.

Moreover, even though the graphene layer is highly perforated, the edges of the holes bind strongly to the metal substrate and thereby prevent the escape from under graphene.

We show that the phenomenon also holds for ion exposure of hexagonal boron nitride and must therefore be assumed to take place for a broad range of 2D materials.

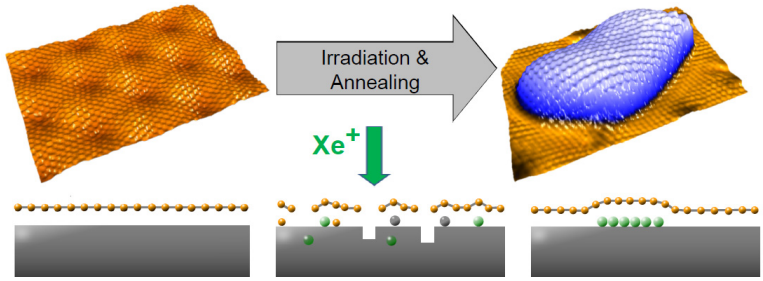

Fig. 1. Schematic of blister formation mechanism in Gr/Ir(111). Top: STM topograph of Gr/Ir(111) before (left) and after ion irradiation with subsequent annealing (right). Bottom:

With scanning tunneling microscopy we image through the hexagonal boron nitride blister lid and find a superstructure corresponding in lattice parameter to what we expect for a crystalline Xe layer. We conclude that due to the strong adhesion of 2D layer to Ir(111) the pressure inside the blisters is in the GPa range.

Finally, we form blisters under a perfect 2D layer by pre-implantation. We envision that the method of energetic particle impingement could be used to trap and react chemical species at very high pressures and temperatures. Since atomically thin layers are transparent to light, one might even study photochemical reactions. Such an approach could also be used for reactive growth of interfacial layers in between the substrate and a 2D layer.

Interfacial Engineering of Electronic and Magnetic States in Complex Oxide Heterostructures by Pulsed Laser Deposition Technique

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In condensed matter physics, exploring new collective quantum states is one of the most essential and fundamental tasks. Towards this goal, establishing heterostructures from complex oxide constituents has been considered as a powerful and promising approach. However, even though theorists have designed and studied extensive heterostructures, it is always challenging to experimentally stabilize many of them during the layer-by-layer synthesis since the existing mismatches tend to lead thermodynamically unfavorable. In this work, we focus our studies on two of the complex oxide systems: transition metal titanates and transition metal nickelates, to show that using the state-of-the-art epitaxial thin film fabrication techniques, it is capable of both tailoring and exploring interesting emergent ground states by means of interfacial engineering approaches.

Novel two-dimensional electron gas system in $YTiO_3/CaTiO_3$ heterostructures.

We present the layer-by-layer growth of high quality $YTiO_3/CaTiO_3$ superlattices using pulsed laser deposition technique, which exhibit interfacial metallic conduction. The crystallinity, surface morphology, film thickness and superlattice structure have been confirmed by *in-situ* high-pressure RHEED (reflection high energy electron diffraction), atomic force microscopy, X-ray reflectivity and X-ray diffraction. The electrical transport measurements reveal that the superlattices maintain metallic from 300 K down to the base temperature while individual $YTiO_3$ (YTO) and $CaTiO_3$ (CTO) single layers grown under the same condition as the superlattices are insulating. Furthermore, the Hall measurements demonstrate the electrons serve as the charge carriers in the superlattices. Temperature dependence of the carrier density as well as the carrier mobility is estimated based on the obtained Hall coefficient.

Artificial Mott state in grapheme-like $NdNiO_3/LaAlO_3$ heterostructures.

We report on the electronic and magnetic properties of the (111)-oriented $2NdNiO_3/4LaAlO_3$ (2NNO/4LAO) superlattices. The layer-by-layer growth of the superlattices was monitored by *in-situ* RHEED. *Ex-situ* X-ray diffraction and HAADF-STEM (high angle annular dark field - scanning transmission electron microscopy) confirmed the (111) bilayer structure of the NNO. Synchrotron based X-ray resonant magnetic scattering (XRMS) measurements demonstrated the magnetic correlations between the Ni sites on this grapheme-like lattice is antiferromagnetic. In addition, the combination of resonant X-ray linear dichroism spectra and first-principle GGA + U calculations reveal the presence of an antiferro-orbital ordering pattern, which has not been observed before in any rare-earth nickelates.

Electronic structure and first order structural transition of $LuFeO_3$

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Hexagonal $LuFeO_3$ is a multiferroic material that exhibits spontaneous electric and magnetic polarizations simultaneously [1]. The electronic structure of hexagonal and orthorhombic $LuFeO_3$ thin films has been systemically studied. The surface termination and the nominal valence states for hexagonal $LuFeO_3$ thin films grown on Al_2O_3 (0001) substrates were characterized by angle resolved x-ray photoemission spectroscopy (ARXPS) [2]. The Lu 4f, Fe 2p and O 1s core level spectra indicate that both the surface termination and the nominal valence depend on surface preparation, but the stable surface terminates in a Fe–O layer. This is consistent with the results of density functional calculations.

The conduction band electronic structure of hexagonal and orthorhombic $LuFeO_3$ thin films have been measured using x-ray absorption spectroscopy (XAS) at iron L edge and oxygen K edge [3]. Dramatic differences in both the spectral features and the linear dichroism are observed. These differences in the spectra can be explained using the differences in crystal field splitting of the metal (Fe and Lu) electronic states and the differences in O 2p-Fe 3d and O 2p-Lu 5d hybridization. Segregation of the hexagonal and orthorhombic phases has been identified by X-ray Photo-electron Emission Microscopy (X-PEEM) [4], indicating that the hexagonal to orthorhombic phase transition includes co-existence of phases.

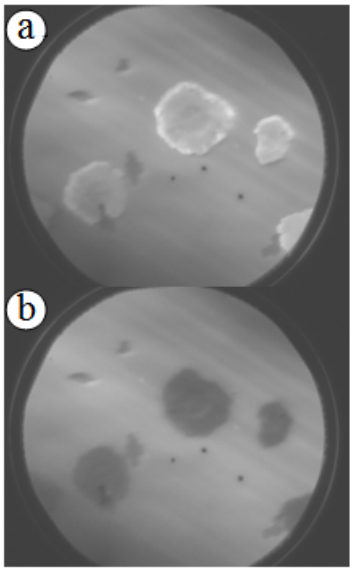

Figure 1. X-PEEM images of $LuFeO_3$ film. (a) and (b) were taken at photon energies of 710 eV and 709 eV respectively with *s* polarization linear X-ray. The "omelet" shape domain indicates the phase segregation of the hexagonal and orthorhombic phases of $LuFeO_3$.

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Session 5 notes:

Hidden Phases of of Double-layered $Sr_3(Ru_{1-x}Mn_x)_2O_7$ Exposed at the Surface

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Double-layered $Sr_3Ru_2O_7$ has received prodigious attention as it exhibits a plethora of exotic phases when perturbed. New phases emerge with the application of pressure, magnetic field, or doping. Here we show that creating a surface is an effective way to reveal hidden phases that are different from those seen in the bulk by investigating the surface properties of $Sr_3(Ru_{1-x}Mn_x)_2O_7$. Using a multitude of experimental techniques (low energy electron diffraction and high resolution electron energy loss spectroscopy) we found out the surface of $Sr_3Ru_2O_7$ is insulating and presumably antiferromagneticaly ordered while the bulk is metallic. In contrast, the surface of $Sr_3(Ru_{0.84}Mn_{0.16})_2O_7$ is metallic while the bulk is insulating. These unusual properties are intimately coupled with the surface structure. The comparison of the bulk and surface phase diagram is shown in Fig. 1.

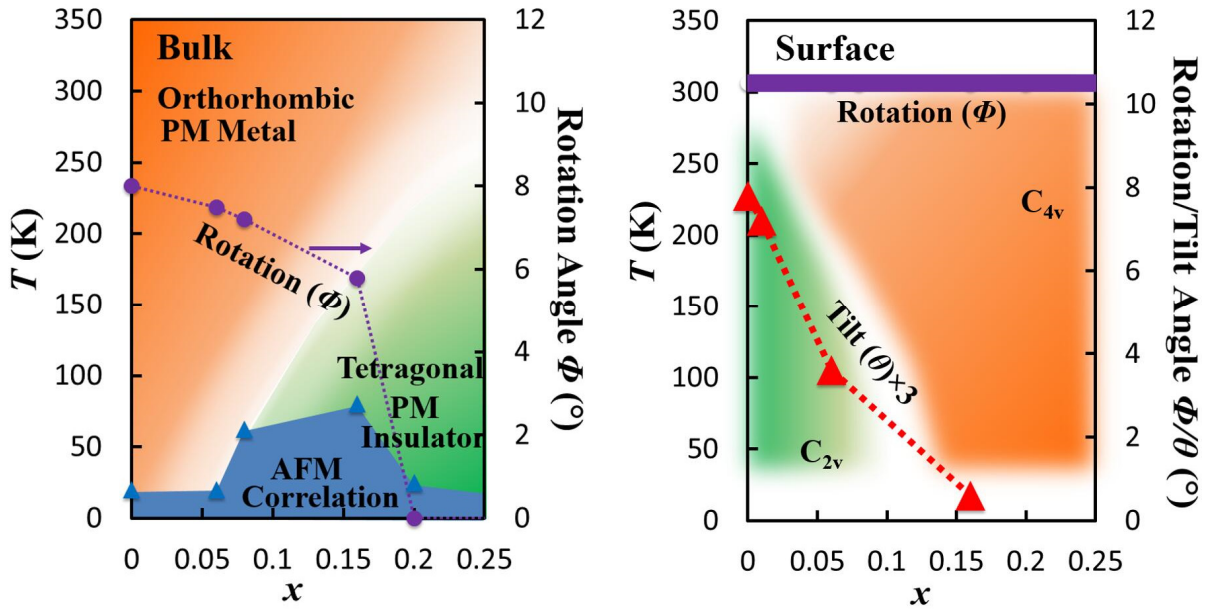

Fig. 1. Comparison of the bulk and surface phase diagram of $Sr_3(Ru_{1-x}Mn_x)_2O_7$. (Left) Bulk phase diagram reproduced from [4]. The insulating phase becomes more dominate as the doping percentage increases while the octahedral rotation decreases at the same time. (Right) Surface phase diagram with the rotation and tilt. The surface has opposite metallicity compared to the bulk.

Electronic Phase Control in Electrolyte-Gated Correlated Oxides

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Phase transitions induced by carrier concentration changes in bulk complex oxides are conventionally achieved by chemical doping. Electrolyte-gated field-effect transistors (FET) based on complex oxides enable one to dynamically control phase transitions in a reversible manner when working with thin film oxides.

Recent experiments, however, raises concerns whether the emergent properties in these FETs originate from pure electrostatic effects or electrochemical reactions, because the response of such devices often far exceeds what one would expect from simply the screening length of the channel. In this presentation, we will present results on our studies on ionic liquid gated correlated oxides such as vanadium dioxide (VO_2) and rare earth nickelates ($RNiO_3$).

It will be shown that channel conductance modulation by the gate voltage can be due to electrostatic or electrochemical doping operating at different time scales. The differences in the time constant of the charging of the gate capacitance and that of conductance modulation can be used to identify fundamental mechanisms involved. We will then present on-going studies to quantify the field effect phenomena to build small signal circuit models for such transistors. With graphene as an inert barrier, we will show how emergent conduction at an electrolyte gate-oxide interface can be deterministically controlled by suppressing electrochemical instability.

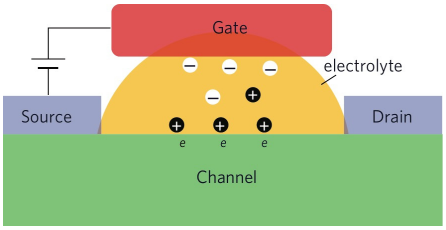

Fig. 1. A schematic of electrolyte-gated field effect transistors based on correlated oxides.

In electrolyte-gated $RNiO_3$, it will be shown that electron doping by the electrochemical reactions lead to a filling-controlled Mott transition that shows a colossal resistivity change that is more than eight orders of magnitude, showing that electrolyte gating can be a power tool to explore the phase diagrams of strongly correlated oxides.

The non-electrostatic effect can be reversible but hysteretic, leading to potentially interesting applications in memory and neuromorphic devices. These studies reveal the crucial role of compositional control in our understanding of emergent behavior at complex oxide interfaces.

Effect of Ligand Exchange with Mercaptoacetic Acid on the Photoresponsivity of Near-IR Photodetectors Based on PbSe Nanocrystals

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Lead selenide (PbSe) nanocrystal has emerged as a potential candidate for detecting light in the near-infrared region. They have interesting optical properties including large Bohr exciton radius and narrow bandgap energy. Depending on the size of PbSe nanocrystals, their bandgap can be tuned to cover the entire near-infrared region. Typically, the synthesized nanocrystals are capped with long organic ligands that act as potential barriers, hampering the charge transportation. Therefore ligand exchange should be performed on the synthesized nanocrystals to replace the original insulator ligands. Previous reports focused on ligand exchange on PbSe nanocrystals using organic capping ligands, such as, oleic acid, ethanedithiol, and butylamine [1,2]. In this research, we propose a ligand exchange procedure using mercaptoacetic acid (MAA) as the new ligands. Near-infrared photodetectors will be fabricated from the PbSe nanocrystals capped with MAA. The PbSe nanocrystals will be synthesized using hot injection technique and characterized by measuring the optical absorption and the photoluminescence. The bandgap of the synthesized nanocrystals will be tuned into the near-infrared region (0.77 eV) by controlling the size of the synthesized nanocrystals, which can be done by controlling the growth time of the nanocrystals. The near-infrared photodetectors will be fabricated by depositing the PbSe nanocrystals on interdigital electrodes using spin coating. The interdigital electrodes will be prepared on a glass substrate using optical photolithography and the evaporation of Ti adhesive layer and Au top contact. The fabricated near-infrared photodetector will be characterized by measuring the current-voltage (*I-V*) characteristics and the spectral response. The *I-V* characteristics of two devices fabricated from PbSe nanocrystals capped with oleic acid and MAA are plotted in Fig. 1.

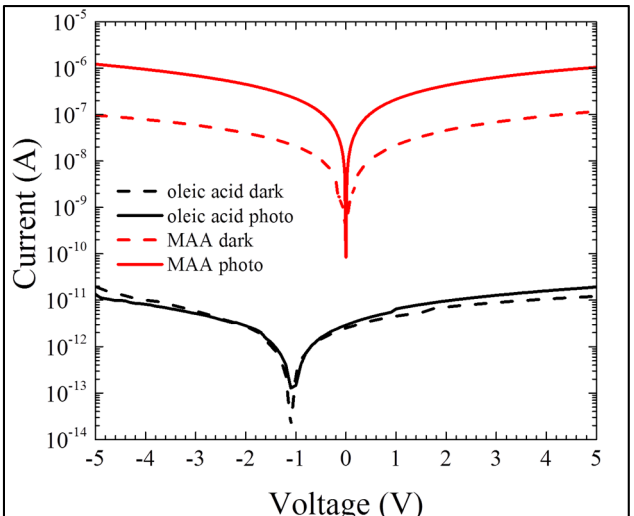

Fig. 1 *I-V* characteristics for photodetectors fabricated from PbSe nanocrystals capped with oleic acid and MAA.

References:

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Exploring Intermolecular Interactions by Imaging Single Bonds with the Scanning Tunneling Microscope

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Compared to intramolecular interactions, intermolecular interactions are relatively weak but they lay the foundation for the research involving molecular recognition, self-assembly and surface adsorption in chemical and biological systems. Measurements of intermolecular interaction at the single molecule level are highly desirable not only to facilitate direct comparison with theoretical calculations but also to reveal the rich local information which otherwise are hidden upon averaging in ensemble measurements, such as the molecular structure, orientation and coupling to the neighboring environment.

Here we demonstrate the quantitative characterization and real space visualization of intermolecular interactions at the single bond level from three different approaches with a sub-Kelvin scanning tunneling microscope (STM). First, the intermolecular interaction can be directly evaluated by measuring the coupled vibrational mode of two interacting molecules with STM inelastic electron tunneling spectroscopy (IETS). Second, the molecular structure and orientation can be imaged by the inelastic tunneling probe (itProbe) [1] based on STM-IETS. In itProbe, a carbon monoxide (CO) molecule is transferred onto the STM tip, as illustrated in Fig. 1A. The energy and intensity of the hindered translation of the CO-tip vary when it is positioned over different locations of an adsorbed molecule and between molecules, such as in the self-assembled hexafluorobenzen (C_6F_6) island. By recording the spatial variations of the intensity due to the energy shift, the geometric structure of each C_6F_6 and intermolecular interactions can be imaged in real space (Fig. 1B). Third, combining itProbe and IETS, the adsorption configuration of physisorbed benzene (C_6H_6) on inert metal surface can be precisely determined and the binding strength can be assessed from the detection of external vibrational modes of benzene.

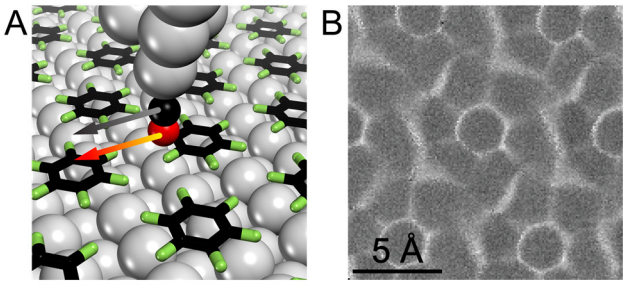

Fig. 1. (A) Schematic of itProbe technique. (B) Bonding structure of self-assembled C_6F_6 island on Ag(110) obtained by itProbe.

References:

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INVITED TALK:

Mechanical engineering considerations for advanced application CPUs

Jonathan W. Thibado

Principal Engineer Intel Corp.

Intel Corporation's Data Center growth is accelerating due to the explosive demand from social media and cloud services. The challenges to the mechanical engineering aspects of this growth is understanding the related physical and environmental considerations. This presentation is meant to share with the audience the trends and concerns at Intel and showcase how our mechanical team addresses these issues with illustrative examples. Through these, similarities and differences between academic research and industry research and development will be highlighted. Time permitting, I will discuss Intel's approaches in designing data center needs for the future.

Session 6 notes:

Core level shifts of doped graphene

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Shifts in the binding energy of core electrons are used in X-ray photoelectron spectroscopy (XPS) to identify changes in the chemical environment of the atoms under concern. In the context of our work, core level shifts (CLSs) of the carbon 1s photoelectrons in graphene (Gr) are monitored to investigate and control intercalation processes or chemical reactions under Gr [1]. Intercalation, i.e., the insertion of atoms or molecules in between Gr and the underlying substrate is a means of decoupling the Gr from its substrate, and to shift the Dirac cone of Gr with respect to the Fermi level without destroying it through strong hybridization [2,3].

By measuring core level shifts for a number of structurally well-defined intercalation layers (O, H, Eu, Cs, see Fig. 1), and comparing with data of decoupled Gr from the literature, we find that the CLS is a non-monotonic function of the doping level. For small doping levels the CLSs are well described by a rigid band model. However, at larger doping levels, a second effect comes into play that is proportional to the transferred charge and counteracts the rigid band shift.

Striking confirmation for this relation between CLS and doping level comes from doping with Li, since for Li no phase separation takes place upon intercalation, and the doping level can be tuned continuously.

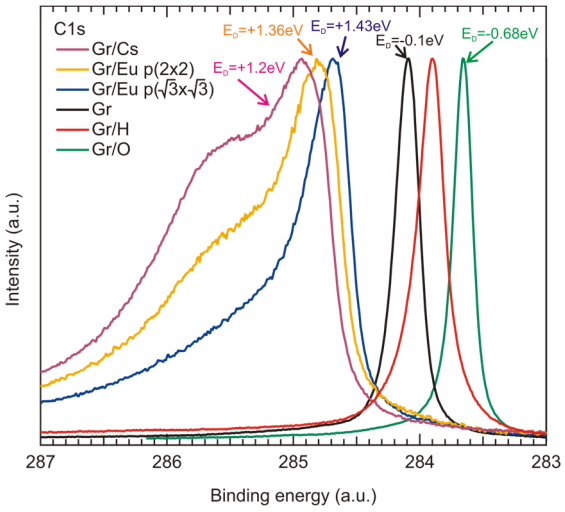

Fig. 1. XP spectra of the C 1s region from right to left of Gr/Cs-p($\sqrt{3} \times \sqrt{3}$)R30°/Ir(111) (magenta), Gr/Eu-p(2×2)/Ir(111) (orange),

Gr/Eu-p($\sqrt{3} \times \sqrt{3}$)R30°/Ir(111) (blue), Gr/Ir(111) (black), Gr/H-p(1×1)/Ir(111) (red) and Gr/O-p(2×1)/Ir(111) (green). Doping levels E_D are indicated next to the curves. For Gr/H/Ir(111) the doping level has not been measured.

References:

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Coupling Organic Molecules to Topological Insulators

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Topological insulators (TIs) are a prime candidate for spintronics application due to their spin-textured surface states on a bulk insulating material.[1, 2] These topological surface states (TSS) are protected by time-reversal symmetry making them robust against defects and perturbations that preserve this symmetry.[3] Modification of the magnetic and electronic properties of TIs has mainly focused on the technique of bulk or surface doping leaving room for organic molecules to control TIs. The organic-TI interface is a unique opportunity to probe the coupling of organic molecules to a bulk insulating material with a spin-momentum locked surface state.

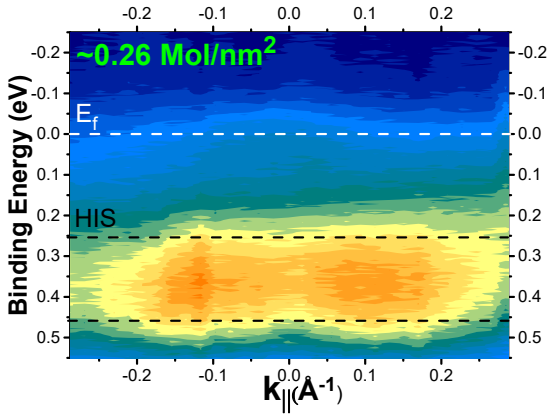

Fig. 1. ARPES of MnPc/Bi_2Te_3 interface showing a new weakly dispersing and wide bandwidth hybrid-interface state.

Through a combination of spatially-averaged (ARPES) and local probing (STS) of electronic states, we show the emergence of a new HIS for MnPc adsorbed on Bi_2Te_3 and show it to be localized at the molecular adsorption site. We suggest that this interface system may have important implications for understanding the role of local time reversal symmetry breaking in TI's and in controlling spin injection into these novel materials.

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Surface Reactivity of Pt-Cu(111) Single Atom Alloys: Model Studies that Guide the Design of Atom Efficient Pt Nanoparticle Catalysis

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Platinum is a ubiquitous catalyst in the chemicals and energy production sectors, however, its scarcity in nature and high price will limit future proliferation of current and new Pt-catalyzed reactions. One promising approach to conserve Pt involves understanding the minimal number of Pt atoms needed to catalyze a desired reaction and then designing catalysts with the smallest necessary Pt ensembles. Guided by surface chemistry and microscopy studies we designed and tested a new generation of Pt/Cu nanoparticle catalysts for the selective hydrogenation of butadiene to butene, an industrially important reaction. An isolated Pt atom geometry enables H_2 activation and spillover but is incapable of C-C scission that leads to loss of selectivity and catalyst deactivation. Pt-Cu(111) alloys with ~1 % Pt were found to exhibit high activity and selectivity for butadiene hydrogenation to butene under mild operating conditions. Furthermore, we demonstrate that the single atom alloy (SAA) strategy applied to Pt reduces the binding strength of CO while maintaining catalytic performance. By using surface sensitive studies, we accurately determined the binding strength of CO to different Pt ensembles, and this in turn guided the preparation of Pt-Cu alloy nanoparticles who maintain high hydrogenation activity in the presence of CO.

Synthesis and Characterization of MoS_2 thin films by Pulsed Laser Deposition for Electronic Applications

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Thesis adviser: Manuel A. Quevedo-Lopez[†]

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Two-dimensional materials such as graphene and MoS_2 have been the focus on intense research in last five decades. The common method of exfoliating from layered crystals does not result in large area suitable for many applications. Here, we report the fabrication of several layer MoS_2 films in 50.8mm sapphire substrates using Pulsed Laser Deposition (PLD). To develop this process we fabricated three different targets with sulfur excess (50 % MoS_2, S 50%): I, II, and III with relative densities of 88.13%, 88.665% and 99.99%. The thinnest MoS_2 thin film was 1.33 nm thick (approximately two monolayers) with a roughly Mo/S ratio of 0.5 through all its thickness. Furthermore, this thin film showed a resistivity of $1.54x10^4$ Ω cm which can be attributed to the homogeneity of the Mo and S stoichiometry.

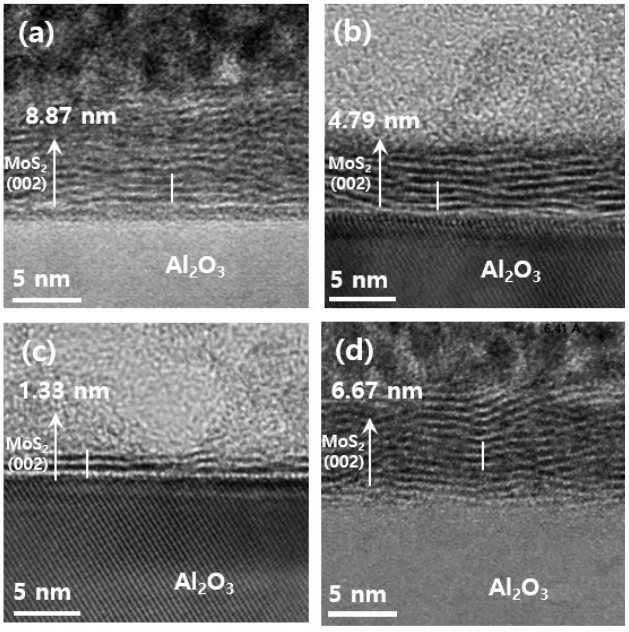

Figure 1. Transmission electron microscopy (TEM) for the MoS_2 films deposited from the different targets. Regardless of the target, pulsed laser deposition allows deposition of layered MoS_2 films on sapphire. Figure 1c shows than one to two layers can also be achieved. Although all the films were deposited under the same PLD conditions there is a clear difference in thickness. This difference is likely due to several target densities. Target 1 (a), Target II(b), Target III (c), Target T (d)

Zinc(II) Tetraphenylporphyrin on Ag(100) and Ag(111): Multilayer Desorption and Dehydrogenation

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The interaction between zinc(II) tetraphenylporphyrin (ZnTPP) molecules and the Ag(100) and Ag(111) surfaces is investigated using a combination of scanning tunneling microscopy as a local probe of the molecular adsorption configuration and x-ray, ultraviolet and inverse photoemissions as probes of the electronic structure. For each surface, a monolayer of ZnTPP, formed by multilayer desorption, exhibits a highly ordered structure in registry with the underlying surface lattice. Subsequent annealing leads to a transition from intact molecular adsorption to dehydrogenation and subsequent rehybridization. This rehybridization is both intramolecular, with a flattening of the molecules and a measurable alteration of the electronic structure, and intermolecular leading to 2D-growth of extended covalently bound structures. The formation of covalent bonds upon annealing intact TPP molecules, shown as Figure 1, is a relatively new frontier and has broad implications on the creation of highly ordered 1D or 2D structures through direct chemical reactions at the surface. Self-assembled TPP monolayers exhibit extremely low defect densities and high order over many tens or hundreds of nanometers with their intermolecular interactions dictated by phenyl-phenyl van der Waals forces. However van der Waals interactions lead to fragile structures with weak intermolecular attraction. The formation of covalent bonding could in principle alleviate these drawbacks, and ideally one could take the long-range self-assembled structure created via weaker interactions and lock it in place using covalent bonding, resulting in a rigidly-connected 2D structure. Thus, intermolecular bonding through hydrogen loss indicates a possible route for long-range 2D polymer growth.

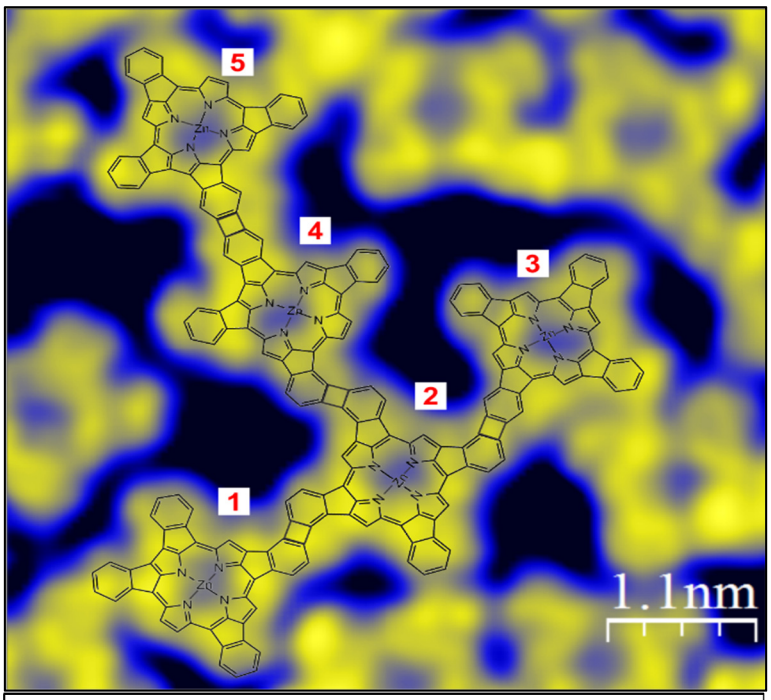

Figure 1. STM image of dehydrogenated ZnTPPs on Ag(100) after annealing to 640K. A chain of covalently bonded molecules is shown comprised of several rehybridized ZnTPPs due to dehydrogenation.

Session 7 notes:

Electrical Control of Chiral Phases in Electrotoroidic Nanocomposites

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This work [1] uses a first-principles-based effective Hamiltonian to study room-temperature optical properties of electrical vortices in the electrotoroidic nanocomposite introduced in [2]. These vortices exhibit order parameter of electrical toroidal moment. Electrotoroidic systems with parallel electrical polarization and toroidal moment can be chiral and thus exhibit optical activity [3], or rotation of the plane of linearly polarized light by a fixed amount per unit length characterized by gyrotropy tensor g_{mk}. This work considers electrical control of chiral phases and enhancement of gyrotropy in such a system. Combining molecular dynamics (MD) and Monte Carlo (MC) simulations in our scheme finds optical rotation is maximized at room temperature for some applied DC electric field in our system [1]. This suggests the possibility of novel optical applications of electrical vortices, e.g., electrically-controlled ultrafast optical circulators and isolators in fiber-optic-based devices. Possible extensions of this work include energetics of switching between chiral and non-chiral phases and control of photovoltaic properties.

We consider a periodic square array of $BaTiO_3$ nanowires in a $SrTiO_3$ medium with cross-section 4.8x4.8 nm^2 perpendicular to the wire axis and adjacent wires separated by 2.4 nm. Absent applied electric fields, the system has Curie temperature T_C=240 K and toroidal moment vanishes at T_G=330 K. In [3] using MD, at 15 K by applying a sinusoidal AC electric field along [001] of amplitude 10^9 V/m with frequency between 1 and 100 GHz, optical rotation as much as 0.62 rad/meter at 100 GHz was found. Moreover, gyrotropic coefficient varied with temperature T as $g_{11}=A/[(T_C-T)(T_G-T)]^{1/2}$ for a constant A. A strategy to enhance optical rotation, then, is to make $T_C=T_G$ and let T approach this temperature [1]. MC simulations in which we heated the system under various DC electric fields were used to build a phase diagram to find this critical temperature: room temperature! MD simulations were then used to calculate g_{11}, confirming g_{11} was maximized (double the null field value) at this temperature at the critical field.

R.W. acknowledges this material is based upon work supported by the NSF Graduate Research Fellowship Program under Grant No. DGE-0957325 and the University of Arkansas Graduate School Distinguished Doctoral Fellowship. Y.N., Z.G., and L.B. acknowledge the support of the ARO grant W911NF-12-10085. S.P. and L.B. thank the financial support of the DARPA grant HR0011-15-2-0038 and the Physics Department of the University of Arkansas.

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Spin-Polarized Interfacial Hybridization between different 8-hydroxyquinolates and Cr(001) surface

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As organic materials attract a lot of attention due to their promising applications in spintronic devices, it is realized that spin-polarized interfacial hybridization between organic molecules and magnetic electrode plays an important role to improve performance of organic spintronic devices.[1,2] In order to understand the hybridization mechanism at the interface, spin polarized scanning tunneling microscopy and spectroscopy (SP-STM/STS) is employed to study the electronic and magnetic properties of the interface between single tris (8-hydroxyquinolinato) aluminum (Alq3) molecule and antiferromagnetic Cr(001) surface. Spin-resolved spectra measurement exhibits clear spin-polarized interfacial hybridization between Alq3 and Cr(001). LUMO of Alq3 is partially filled by electrons from bulk sp band of Cr, while the spin-polarized surface state of Cr(001) is retained at molecular adsorption sites. This indirect hybridization results in high spin asymmetry at Fermi level, which could potentially improve spin injection at the interface. Tris (8-hydroxyquinolinato) chromium (Crq3) adsorbed on the same substrate is also studied and compared with Alq3. The hybridization between LUMO of Crq3 and surface state of Cr(001) leads to two spin-polarized interfacial states below and above Fermi level, which is governed by totally different hybridization mechanism than Alq3. Different orbital geometry of Alq3 and Crq3 indicated by DFT calculation is the major reason to determine the hybridization mechanism. This paves a new way to design metal-organic interface in organic spintronic devices by molecular orbital control.

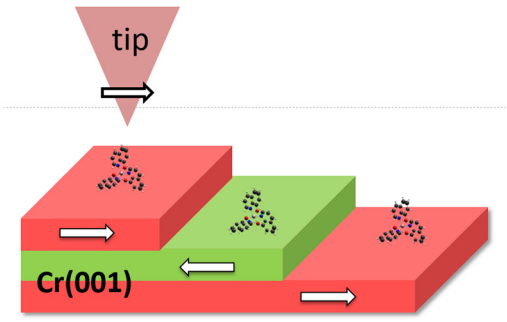

Fig. 1 A schematic diagram of spin-polarized STM measurement on Alq3/Crq3 adsorbed on Cr(001) surface

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Low-dimensional Organics for Electronics Applications

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I will present experimental study on the self-assembly and electronic properties of a spin-crossover complex, $[Fe(H_2B(pz)_2)_2(bipy)]$ on Au(111). The signature functionality for this complex, a low-spin to high-spin transition, arises from a central Fe(II) atom, which is in a d^6 configuration in a (pseudo)octahedral N_6 environment. This Fe(II) atom can be switched between a diamagnetic low-spin (S=0) and a paramagnetic high-spin (S=2) state by external stimuli such as temperature, pressure, light and electric field. Spintronics application that exploit the spin-dependent properties on the molecular level requires that the molecules are in contact with metal electrodes, where interactions may not only determine the spin-dependent functionality of the molecular structures, but also their integrity on the substrate.

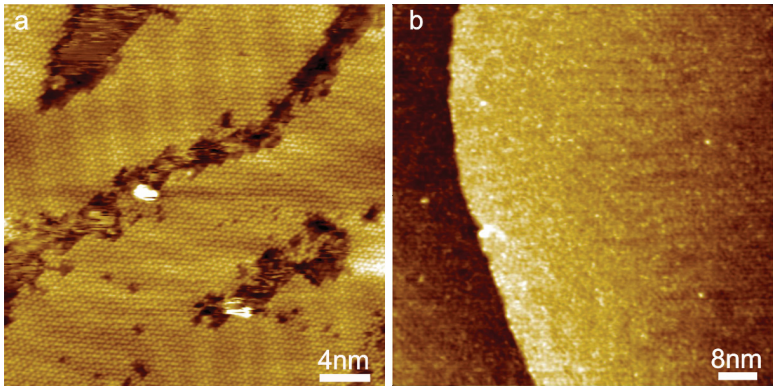

Fig. 1. (a) A bilayer film on Au(111) (b) A 7±3 monolayer film on

I studied ultrathin films of $[Fe(H_2B(pz)_2)_2(bipy)]$ on gold single crystal surfaces, a common electrode material, with variable temperature scanning tunneling microscopy, as a function of film thickness. I was able to show that structural ordering in the bilayer coverage is thermally induced; a particular bilayer stacking described earlier by D. Dougherty [1] is established as the films are cooled well below their spin transition temperature, and this ordering is maintained when the films are brought back to room temperature.

Importantly, this rearrangement of the molecules is not without consequences for their magnetic properties, as my comprehensive spectroscopic studies that included core-level XPS, angle-resolved XPS and X-ray absorption showed. The dense packing of the molecules in the ordered layers induces conformational changes, which inhibit thermally induced transitions of the molecular spin state, so that both high-spin and low-spin states are preserved far beyond the spin transition temperature of free molecules.

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[1] A Pronschinske, 2013, Chem. Comm., 49, 10446

Van der Waals Epitaxy of WSe_2 Based Heterostructures: A Study of Controlled Nucleation and Grain Morphology

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Transition metal dichalcogenides (TMDs) are 2-dimensional, layered materials with composition and thickness dependent electronic properties. Due to the weak van der Waals interactions between adjacent layers, TMDs enable heterostructure growth with relaxed criterion for lattice matching, allowing the selection of materials based primarily on their electronic properties and quantum mechanical effects. Among these materials, WSe_2 is one of the most interesting TMDs due to its band alignment and carrier effective mass. In this work, we present our recent investigation into the physics and chemistry of nucleation, 2D growth, grain size, and grain shape of WSe_2 on other inert van der Waals substrates. We demonstrate high-quality, crystalline WSe_2 thin films and show how the van der Waals interactions allow for heteroepitaxy of significantly lattice-mismatched materials without strain or misfit dislocations. Yet, at the same time, the VDW interactions are strong enough to cause rotational alignment between the epi-layer and the substrate, which plays a key role in the formation of grain boundaries. To suppress nucleation and grain boundaries and enhance larger area 2D growth, the complex interaction between the W flux, Se flux, and diffusion rates was investigated. W flux and substrate temperature primarily govern the competition between the attachment and diffusion rates and are critical to controlling the WSe_2 nucleation and grain shape as seen in Fig. 1. The growth mode is primarily affected by the Se:W flux ratio which, in conjunction with lower nucleation rates, allows for larger 2D grain growth.

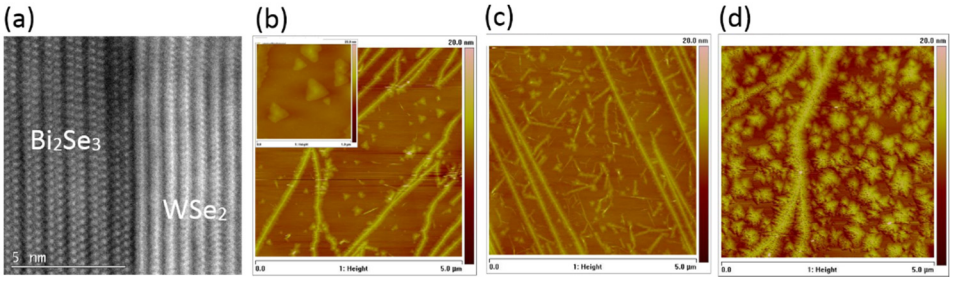

Figure 1. (a) TEM image of WSe_2 on Bi_2Se_3, indicating WSe_2 layered structure and atomically abrupt interface, AFM images of WSe_2 growth on HOPG show (b) triangular grain shapes under equilibrium conditions, (c) “nanorod” like grain shapes under lower substrate temperature and (d) fractal shapes under higher W flux. This demonstrates the impact of W flux and substrate temperature on the resultant grain morphology.

Layer-by-layer interrogation of $La_{2/3}Sr_{1/3}MnO_3$ films on $SrTiO_3$ (001)

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We report on our study of the chemical composition with atomic layer precision in the ultrathin films of $La_{2/3}Sr_{1/3}MnO_3$ (LSMO) grown on $SrTiO_3$ (001), using a combination of *in*- and *ex-situ* microscopy and spectroscopy. Our results reveal that there is substantial increase in the Sr concentration from its bulk value both at interface and surface. Such layer-by-layer variation in composition results in an immense impact on the physical properties of the epitaxial films and heterostructures. It naturally explains the existence of 'dead' layer and the persistent nonmetallic behavior near the surface and interface of LSMO films, regardless their thickness, which are determined by film conductivity and scanning tunneling spectroscopy.

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Characterization of a gate-defined double quantum dot in a Si/SiGe nanomembrane

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We report the characterization of a gate-defined double quantum dot formed in a Si/SiGe nanomembrane [1]. Previously, all heterostructures used to form quantum dots were created using the strain-grading method of strain relaxation, a method that necessarily introduces misfit dislocations into a heterostructure and thereby degrades the reproducibility of quantum devices. Using a SiGe nanomembrane as a virtual substrate eliminates the need for misfit dislocations but requires a wet-transfer process that results in a non-epitaxial interface in close proximity to the quantum dots. We show that this interface does not prevent the formation of quantum dots, and is compatible with a tunable inter-dot tunnel coupling, the identification of spin states, and the measurement of a singlet-to-triplet transition as a function of the applied magnetic field.

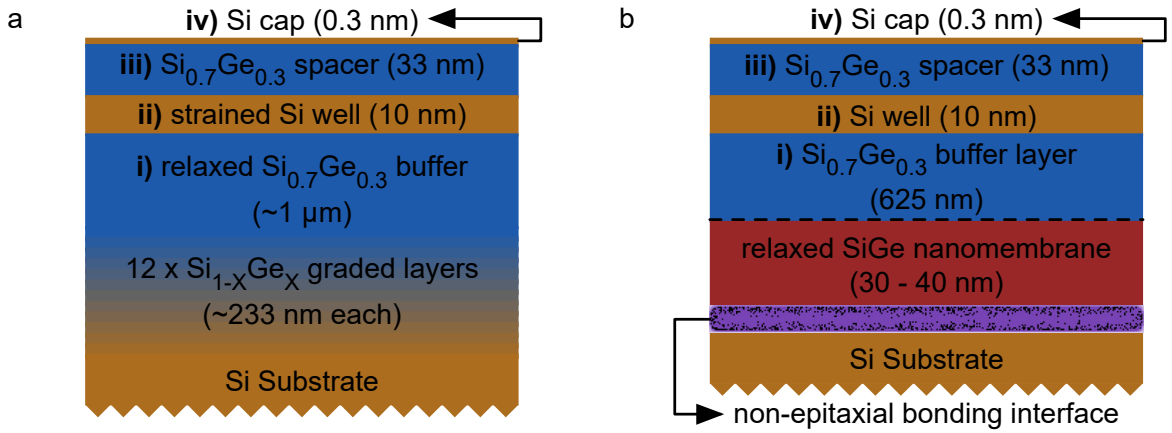

Fig. 1 (a) schematic diagram of typical heterostructure formed using strain-grading techniques. (b) Schematic depiction of a heterostructure formed via liquid release of a nanomembrane.

This work was supported in part by ARO (W911NF-12- 0607), NSF (DMR-1206915, PHY-1104660), and the Department of Defense. The views and conclusions contained in this document are those of the authors and should not be interpreted as representing the official policies, either expressly or implied, of the US Government.

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Session 8 notes:

Synthesis of Two-Dimensional MoS_2 by a CVD Process

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Two-dimensional single and few layers of MoS_2 have been attract much attention due to their unique property and potential for applications. Synthesis of large area MoS_2 on substrate will lead to possible device fabrication. In this study, large area MoS_2 of high crystallinity and large size were synthesized by a Chemical Vapor Deposition process. Both triangle-shape-flake and continuous film of monolayer and multilayer MoS_2 were obtained. Analysis of layer roughness, size, thickness, uniformity and crystallinity were studied by optical microscope, AFM, SEM, and Raman. The effects of precursor concentration, pressure in chamber, gas flow rate and plasma treatment on MoS_2 layer growth were also investigated in order to understand the growth mechanism of triangle-shape MoS_2 on SiO_2/Si substrate. Understanding of the initial growth was also achieved by studying the crucial role played by the substrate surface condition in MoS_2 growth. It was found that the right surface condition before deposition is necessary for successful growth while other conditions were kept the same. The study of growth process will eventually help deposit ultra large size MoS_2 layers of wafer scale for applications.

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Reaction of Dysprosium with Graphite Surface: Competition between Carbide Formation and Surface Intercalation

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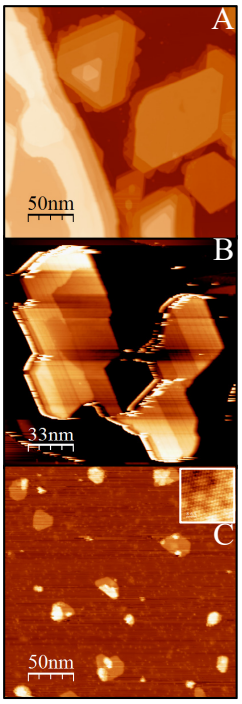
We have studied the interaction of dysprosium with the basal plane of graphite at elevated temperatures using scanning tunneling microscopy (STM). Two types of graphite surfaces are prepared: (1) a pristine graphite surface prepared by tape-cleavage in air and heating in UHV; and (2) a pristine surface treated by argon ion bombardment to produce surface defects. On the pristine surface, deposition of Dy at 750 K results in compact three-dimensional islands (Fig. A), with shapes that can be attributed to growth of close-packed layers of Dy metal. These are quite distinct from the islands that form upon further thermal treatment at 1000 K. This results in striated islands with step edges at angles of 60° and 120° (Fig. B), surrounded partially or completely by etched pits in the carbon substrate. Based on the observation of carbon erosion, we identify the striated islands as dysprosium carbide. The requirement of mass balance of C atoms reveals the stoichiometry of the carbide islands to be Dy_2C, a known bulk carbide. Hence, surface carbide can be readily identified based on its unique morphological features. The second type of graphite surface, prepared by argon ion bombardment, shows less propensity for carbide formation but instead, shows development of a new type of feature. These are 0.6-nm tall islands (Fig. C), often with hexagonal footprints and often emanating from the base of a Dy island. Atomic-scale resolution (inset to Fig. C) of the tops of these islands shows the symmetry and spacing expected for graphite. We propose that these are buried or intercalated Dy islands, covered by one or more layers of graphene. Formation of these islands is strongly promoted by the defects created by ion bombardment, which serve as entry portals for Dy diffusion between graphite galleries.



This work was supported by the US Department of Energy (DOE), Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division through the Ames Laboratory, which is operated by Iowa State University under contract # DE-AC02-07CH11358.

Elucidating the mechanism of heterogeneous acetaldehyde oxidation on polycrystalline platinum through flow cell studies

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Acetaldehyde is a biologically and industrially significant molecule that occurs widely in nature and is utilized as a chemical precursor to several compounds. Due to its widespread industrial use, it is a pollutant of special concern both in the environment and in living- and workspaces. While the platinum-catalyzed oxidation of acetaldehyde in aqueous environments is well-studied[1], little work has investigated the dynamics of this catalytic oxidation reaction in the gas phase. We have previously presented preliminary results of study on this system[2].

We report investigation of the kinetics and dynamics of gas-phase acetaldehyde oxidation over polycrystalline platinum as a function of surface temperature and oxygen coverage using a flow reactor cell. The cell couples use of tunable diode laser absorption spectroscopy to probe the rotational vibrational state distribution of product CO_2 with quadrupole mass spectrometry to monitor reaction kinetics. Previous work in our group has used this approach to study the catalytic oxidation of carbon monoxide and methanol, among other molecules[2,3].

Results indicate that production of CO and CO_2 proceeds via two distinct pathways. Acetaldehyde adsorbed on the surface decomposes to acetyl, which in turn decomposes to CO and CH_x. The adsorbed CO so prepared desorbs to yield the bulk of CO generated across all reaction conditions and also yields CO_2 with a relatively deactivated asymmetric stretching mode under conditions of high temperature and low oxygen coverage. The acetyl-derived CH_x dehydrogenates to yield surface carbon and H adatoms. Total oxidation of this surface carbon is the primary source of CO_2 and is found to yield products with a preferentially excited asymmetric stretch. Combination of the CH_x-derived H adatoms with surface O drives production of water.

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Adsorption of Ammonia and Water on Metal-supported Iron Phthalocyanine

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The ability to control and manipulate structures of single molecules by external means is desirable for applications in molecular electronics, spintronics, catalysis and molecular sensors. Understanding the interaction of adsorbed ligands on single molecules is necessary to design these systems. This work was inspired by theoretical calculations predicting a 0.9 Å displacement of the iron centres of FePc on the Au(111) surface upon ligation of ammonia[1], as well as by experimentally observed electronic changes indicative of the "surface *trans*-effect"[2]. Using dispersion corrected Density Functional Theory (DFT) calculations, we show that ligation of ammonia and water to iron phthalocyanine (FePc) on Ag(111) increases the adsorption height of the central Fe atom by 0.19 and 0.07 Å, respectively, both of which agree very well with the recent X-ray standing waves measurements[3]. The significantly reduced atomic displacement is caused by inclusion of derpersion forces through either an semi-empirical method or an non-local exchange-correlation functional. Moreover, the calculated charge redistribution induced by water adsorption shows an accumulation of charge between the surface, the Fe atom and the ligands along the σ-bonding direction, similar to the redistribution caused by ammonia. The observed structural and electronic change can be explained by "trans effect" induced by ligand substitution in coordination complexes. This result has wide-ranging implications in the field of metal-organic complexes supported on metal substrates.

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Anomalously Deep Polarization in $SrTiO_3$(001) Interfaced with an Epitaxial Ultrathin Manganite Film*

Zhen Wang[1, 2], Jing Tao[2], Liping Yu[3], Hangwen Guo[1], Lina Chen[1], Myung-Geun Han[2], Lijun Wu[2], Huolin Xin[2], Kim Kisslinger[2], E. W. Plummer[1], Jiandi Zhang[1], and Yimei Zhu[2]

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The last couple of decades witnessed the discovery of extraordinary phenomena at the interface of transition metal oxides (TMOs). Materials interfaced with $SrTiO_3$ (STO) create a lot of intriguing interfacial phenomena, from 2D electron gas to novel superconductivity [1-2]. While very few focus on the roles of structural relaxation/distortion, especially those from the substrate in the vicinity of the interface. Using atomically-resolved scanning transmission electron microscopy (STEM) imaging and electron energy loss spectroscopy (EELS), we reveal a remarkably deep polarization in non-ferroelectric STO near its interface with an ultrathin nonmetallic film of $La_{2/3}Sr_{1/3}MnO_3$. The polarization in STO extends about 20 unit cells from the interface, with an averaged value of ~ 21 $\mu C/cm^2$. Moreover, we observed an electric field near the interface in STO, pointing towards the interface, by electron holography. Combining our experimental results with first principles calculations, we propose that the observed deep polarization in STO is induced by the electric field originating from oxygen vacancies that extend beyond a dozen of unit-cells from the interface. These intriguing effects in STO may inspire researchers to further pursue studies of emergent interface properties by probing the effects from lattice distortion, and compositional variation microscopically. It also provides important evidence of the role of defects in the novel interface properties of transition metal oxides.

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Session 9 notes:

Titania Containing Thin Films for the Detection of TATP and Peroxide Vapors

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Titania nanoparticles in a hydroxypropyl cellulose matrix produced using a sol-gel method were utilized to prepare coatings on cellulose paper, glass microfibers, and silica. The exposure of these materials to hydrogen peroxide gas and TATP vapor leads to the development of an intense yellow color. Using an inexpensive web camera and a tungsten lamp to measure the reflected light, first-order behavior in the color change was observed when exposed to peroxide vapor concentration as low as 50 ppm. However, while being extremely sensitive to hydrogen peroxide vapors, the sol-gel material had low reactivity to TATP vapor, changing color only after an exposure for an hour or more. For TATP, TLC silica plates saturated with on titanyl sulfate dissolved in an acidic ionic liquid were developed and tested. The acid content of the films was extremely important for TATP detection. These new films have led to an extremely sensitive coating which can detect both hydrogen peroxide and TATP vapors in concentrations of a few parts per million within minutes of exposure and are stable for extended periods of time.

Epitaxial Growth of Graphene Nanoribbons on Cu(111)

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Graphene, a two-dimensional carbon allotrope, is often considered as a promising material for electronics applications. However, the absence of an electronic bandgap in graphene prevents its use in logic devices. According to theoretical studies, substantial bandgaps over 1 eV can be found in narrow graphene nanoribbons (GNRs) that have atomically precise armchair edges and widths < 2 nm. Historical methods of producing GNRs have been top-down approaches, and as a consequence were limited by imprecise edges and nanometer resolution. We present a two-step, bottom-up route to atomically precise chevron-shaped GNRs with armchair edges on Au(111) and Cu(111), with thermally driven surface assembly imaged *via* scanning tunneling microscopy (STM), see Fig. 1. The chevron-shaped GNRs possess an electronic band gap of ~ 1.6 eV [1,2], and on Cu(111) their arrangement is observed to be epitaxial, with ribbons preferentially aligning with respect to each other on the metal surface (Fig. 1).

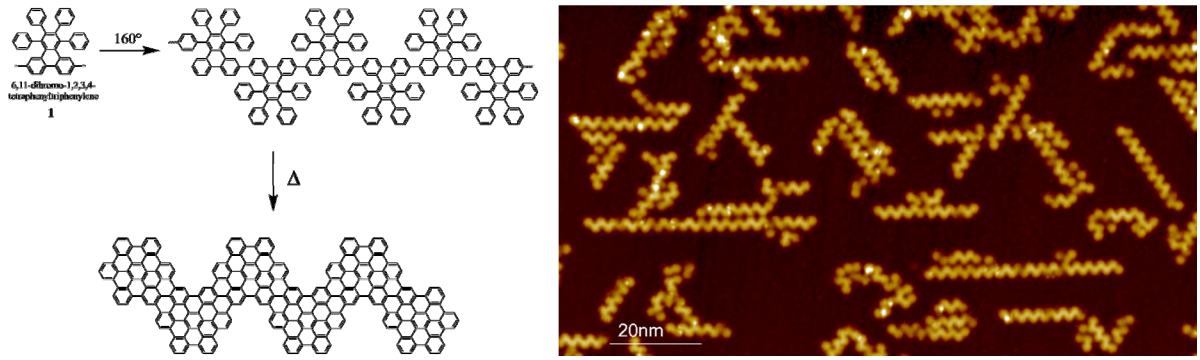

Fig. 1. Left: A schematic for the conversion of precursor **1** to polymer and nanoribbon forms. Right: STM image of chevron nanoribbons on Cu(111).

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Enhanced Photoresponsivity by HIPS-GLAD and SAD-GLAD core/shell nanorod array photodetectors

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A core/shell design can significantly improve the photoresponsivity. In this study, vertically aligned n-type indium sulfide (In_2S_3) nanorods were grown first by glancing angle deposition (GLAD) technique as the core material. Then, these nanorods were coated either with a p-type copper indium sulfide (CIS) shell layer using a high pressure sputtering (HIPS) or silver (Ag) shell by a small angle deposition (SAD) as first and second designs, respectively. It was shown in both cases a uniform conformal shell layer greatly improves the photocurrent and lowers the dark current.

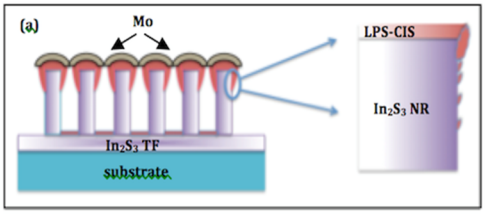
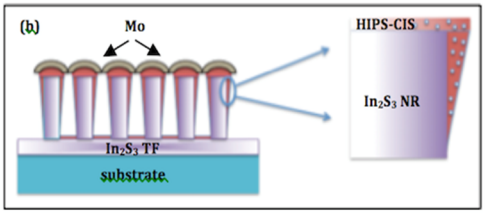


Fig. 1. Schematic illustration of In_2S_3/CIS/Mo core/shell photodetectors whose shell layer was grown by (a) low pressure sputtering (LPS) and (b) high pressure sputtering (HIPS) [1].



We have investigated the effect of working gas pressure of CIS shell layer on photoresponsivity [1]. We observed that HIPS-device has a more uniform conformal CIS shell around core nanorods. As illustrated in Fig. 1, a more uniform core/shell structure results in superior photocurrent (not shown here) for HIPS-CIS devices compared to the ones with conventional low pressure sputtered (LPS) CIS devices that suffers from poor conformality.

Similarly, we have shown in the second design that a conformal SAD Ag layer around the core In_2S_3 nanorods greatly improves the photoresponsivity mainly due to effective collection of photogenerated charge carriers [2].

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[2] H. Cansizoglu et. al., ACS Appl. Mater. Interfaces **6**, 8673−8682 (2014).

The Manipulation and Analysis of ZnO Nanorods with Applications for Photovoltaic Devices

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As the demand for energy increases, nonrenewable energy providers such as coal, gas and oil are not enough to meet the increased demand for energy. In order to alleviate this strain on environment, as well as supplement the oncoming demand, alternative energy sources such as solar need to be incorporated. Typical solar cells made of crystalline silicon are expensive to manufacture and are relatively inefficient at converting light to usable energy[1]. Our research focuses on using materials operating at specific wavelengths of the solar spectrum (the *n*-type thin film nanostructured materials) and developing technologies to manufacture it cheaply while simultaneously increasing its overall conversion efficiency.

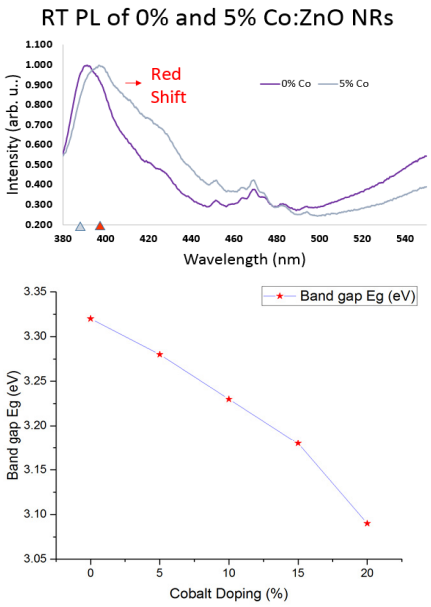

Fig. 1. (Top) A red shift observed using RT PL for cobalt doped ZnO NRs

(Bottom) A change in conductivity observed as the percentage of cobalt doping increases.

Zinc Oxide (ZnO) is a wide bandgap semiconductor that is relatively inexpensive and simultaneously very malleable, making it perfect for photovoltaic applications. ZnO nanorods (NR) can be grown using a low temperature hydrothermal process which increase surface area compared to bulk material and establishes direct channels for electrons to flow[2]. By changing the molar concentrations of precursor materials, as well as the temperature and time which they are grown, we found that we could reproducible control the length and diameter of the nanorods. We also found that by adding dopants into the precursor solution we could change the optical and electrical properties of ZnO nanorods (Fig.1). In this study we employ optical spectroscopy and x–ray diffraction to observe changes in crystal bonding and to prove incorporation of dopants. In addition, we use scanning tunneling spectroscopy to calculate local density of states and photoluminescence (PL) to quantify changes in optical properties of doped ZnO nanorods.

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