RUTGERS
School of Arts and Sciences

# *THIRTY-SECOND ANNUAL SYMPOSIUM*

*of the*

# *LABORATORY FOR SURFACE MODIFICATION/ INSTITUTE FOR ADVANCED MATERIALS, DEVICES AND NANOTECHNOLOGY*

**Tuesday, February 27, 2018**

**8:30 a.m. to 5:00 p.m.**

**Rutgers, the State University of New Jersey**

## PROGRAM

**Life Science Center**
**Busch Campus**
**Piscataway, New Jersey**

RUTGERS
Institute for Advanced Materials, Devices and Nanotechnology

Laboratory for Surface Modification

NanoPhysics Laboratory

# THIRTY-SECOND ANNUAL SYMPOSIUM
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**8:30 Registration, coffee**

**8:55 Introductory Remarks**
**Professor Torgny Gustafsson,**
**Director, Laboratory for Surface Modification**

## SESSION I:

## COMPLEX MATERIALS

**Chair: Professor David Vanderbilt**
**Board of Governors Professor**
**Department of Physics and Astronomy**

**9:00 Nearly Triple Point Topological Phase in Half-Metallic GdN**
Jinwoong Kim, Heung-Sik Kim and David Vanderbilt
*Physics and Astronomy*

**9:15 Gapless Magnetic Excitation from Quantum Antiferromagnetic Chains with Strong Spin-Orbit Coupling**
Mai Ye*[1], Jae-Wook Kim[1], Choong-Jae Won[2,3], Sang-Wook Cheong[1] and Girsh Blumberg[1]
*[1]Physics and Astronomy, [2]Max Planck POSTECH/Korea Research Initiative, Pohang University of Science and Technology and [3]Laboratory of Pohang Emergent Materials, Pohang Accelerator Laboratory*

**9:30 The Axion Insulator Phase in Pyrochlore Iridates**
Nicodemos Varnava* and David Vanderbilt
*Physics and Astronomy*

**9:45 Cluster Dynamical Mean-Field Theory Study of the Deficient Spinel Chalcogenide $GaV_4S_8$**
Heung-Sik Kim, Kristjan Haule and David Vanderbilt
*Physics and Astronomy*

**10:00 – 10:15 Coffee Break and Poster Session**

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## SESSION II:

## NOVEL PHENOMENA AT SURFACES AND INTERFACES

**Chair: Professor Robert Bartynski**
**Chair, Department of Physics and Astronomy**

**10:15** ****HIGHLIGHT PRESENTATION****

**The Exciting New Interface Physics**
**Ivan Božović**
*Brookhaven National Laboratory*

**11:00 Modulation Doping in $LaNiO_3/SrIrO_3$ Superlattices from First Principles**
Michele Kotiuga, Heung-Sik Kim, David Vanderbilt and Karin M. Rabe
*Physics and Astronomy*

**11:15 Defect Formation on the Surface of Giant Rashba Systems**
Wenhan Zhang*[1], Damien West[2], Lunyong Zhang[3], Sang-Wook Cheong[1,4], Shengbai Zhang[2] and Weida Wu[1]
*[1]Physics and Astronomy, [2]Physics, Applied Physics and Astronomy, Rensselaer Polytechnic Institute, [3]Laboratory for Pohang Emergent Materials & Max Planck POSTECH Center for Complex Phase Materials, Max Planck POSTECH/Korea Research Initiative, Korea and [4]Rutgers Center for Emergent Materials*

**11:30 Current-Density Implementation for Calculating Flexoelectric Coefficients**
Cyrus E. Dreyer[1], Massimiliano Stengel[2,3] and David Vanderbilt[1]
*[1]Physics and Astronomy, [2]ICREA-Institució Catalana de Recerca i Estudis Avançats, Barcelona, Spain an d[3]Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Campus UAB, Bellaterra, Spain*

**11:45 An Unusual Example of Kinetically-Trapped Molecular Self-Assembly: ZnTPP on Ag(100)**
Sylvie Rangan[1], Peter Kim[1], Charles Ruggieri[1], Robert A. Bartynski[1] and Steven Whitelam[2]
*[1]Physics and Astronomy and Laboratory for Surface Modification and [2]Molecular Foundry, Lawrence Berkeley National Laboratory*

**12:00 – 1:00 Lunch and Poster Session**

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## POSTER PAPERS:

**1) Characterization of Highly Active Electrodeposited $Li_xCoO_2$ Thin Films for Enhanced OER in PGM-Free Photoelectrochemical Cells**

Ajay Kashi*[1], Shinjae Hwang[2], Anders B. Laursen[2] and G. Charles Dismukes[2]
*[1]Chemical and Biochemical Engineering and [2]Chemistry and Chemical Biology*

**2) Observation of Resonances in the Raman Cross Section of Surface Phonons in on $Bi_2Se_3$, $Bi_2Te_2Se$ and $Bi_2Te_3$**

A. -C. Lee*[1], H.-H Kung[1], S. -W. Cheong[1], R. Merlin[2], I. Boulares[2] and Girsh Blumberg[1,3]
*[1]Physics & Astronomy, [2]Physics, University of Michigan and [3]National Institute of Chemical Physics and Biophysics, Estonia*

**3) Availability of the Elements for Heterogeneous Catalysis – Predicting the Industrial Viability of Novel R&D Catalysts**

Anders B. Laursen[1,2], Jens Sehested[3], Ib Chorkendorff[2] and Peter C. K. Vesborg[2]
*[1]Chemistry and Chemical Biology, [2]Physics at Technical University of Denmark and [3]Haldor Topsoe A/S*

**4) Thermocapillary Multidewetting of Thin Films**

Arielle Marie Gamboa*, Michael Nitzsche, Valeria Saro-Cortes, Tianxing Ma, Lin Lei and Jonathan Singer
*Mechanical and Aerospace Engineering*

**5) Topographical Constraints on the Permeation of Electrosprayed Particles**

Dylan Kovacevich*, Lin Lei and Jonathan P. Singer
*Mechanical and Aerospace Engineering*

**6) Spatially Resolved High-Resolution Core Shell Electron Energy Loss Studies of Interfaces in Semiconductor Devices**

Hongbin Yang*[1], Eric L. Garfunkel[1] and Philip E. Batson[2,3]
*[1]Chemistry and Chemical Biology, [2]Physics and Astronomy and [3]Materials Science and Engineering*

**7) Solution to the Hole-Doping Problem and Tunable Quantum Hall Effect in $Bi_2Se_3$ Thin Films**

Jisoo Moon*[1], Nikesh Koirala[1], Maryam Salehi[2], Wenhan Zhang[1], Weida Wu[1] and Seongshik Oh[1]
[1]*Physics and Astronomy and* [2]*Materials Science and Engineering*

**8) Perovskite-based Oxyhydrides as Potential Ammonia Catalysts**

Joshua Flynn, Martha Greenblatt and Gerard Dismukes
*Chemistry and Chemical Biology*

**9) Selective Electrochemical $CO_2$ Reduction to C3 and C4 Carbohydrates Exceeding 90% Energy Efficiency**

Karin U. D. Calvinhoa*, Anders B. Laursena, Kyra M. K. Yapa, Krishani Teeluck and G. Charles Dismukes
*Chemistry and Chemical Biology*

**10) Mechanistic Studies on Nickel Phosphide Electrocatalysts for the Carbon Dioxide Reduction Reaction**

Krishani M. Teeluck*, Karin U. D. Calvinho, Anders B. Laursen and G. Charles Dismukes
*Chemistry and Chemical Biology*

**11) Titanium Nitride as a Conducting Interfacial Layer Between Hydrogen Evolution Catalysts and Silicon Photocathodes for Stable Solar-to-Hydrogen Water Splitting Devices**

Shinjae Hwang*, Spencer H. Porter, Anders B. Laursen, Hongbin Yang, Mengjun Li, Viacheslav Manichev, Karin Calvinho, Voshadhi Amarasinghe, Martha Greenblatt, Eric Garfunkel and G. Charles Dismukes
*Chemistry and Chemical Biology*

**12) Measuring the Surface Damage of Femtosecond Pulse Radiation by Channeling RBS**

Ryan Thorpe[1], Andrey Baydin[2], Halina Krzyzanowska[2], Thomas Schenkel[3], Norman Tolk[2], Leonard Feldman[1] and Torgny Gustafsson[1]
*[1]Physics and Astronomy and Laboratory for Surface Modification, [2]Vanderbilt University, Nashville, TN and [3]Lawrence Berkeley National Lab, Berkeley, CA*

**13) Rubrene vs Fluorine-Functionalized Rubrene Molecules: Self-Assembly, Electronic Structure and Energy Alignment**

Jonathan Viereck*, Sylvie Rangan and Robert A. Bartynski
*Physics and Astronomy and Laboratory for Surface Modification*

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## SESSION III:

## LOW DIMENSIONAL MATERIALS

**Chair: Professor Leonard C. Feldman**
**Departments of Physics and Astronomy and of Materials Science and Engineering**

**1:00** ****HIGHLIGHT PRESENTATION****

**2D Materials: Surfaces, Interfaces and Defects**
Robert M. Wallace
*Materials Science and Engineering, the University of Texas at Dallas*

**1:45 Chemical Vapor Deposition Growth of Metallic Niobium Disulfide**
Xiuju Song, Yan Wangand and Manish Chhowalla
*Materials Science and Engineering*

**2:00 Indium Contacts for Minimizing Contact Resistance of 2D $MoS_2$ Field Effect Transistors**
Yan Wang *[1], Jieun Yang[1], Xiuju Song[1,2], Fang Zhao[3] and Manish Chhowalla[1]
*[1]Materials Science and Engineering, [2]College of Optoelectronic Engineering, Shenzhen University and [3]Physics, Princeton University*

**2:15 Stripe Quadrupole Order in the Nematic Phase of FeSe**
W.-L. Zhang[1], S.-F. Wu[1], S. Kasahara[2], T. Shibauchi[3], Y. Matsuda[2] and Girsh Blumberg[1,4]
*[1]Physics & Astronomy, [2]Physics, Kyoto University, [3]Advanced Materials Science, University of Tokyo and [4]National Institute of Chemical Physics and Biophysics, Estonia*

**2:30 Correlation of Atomic Scale Defects Using He Ion Beam in 2D $MoS_2$ with Optical, Electronic and Catalytic Properties**
Jieun Yang*[1], Slava Manichev[2,4], Maureen Lagos[1,4], Raymond Fullon[1], Yan Wang[1], Xiuju Song[1], Ibrahim Bozkurt[1], Daniel Kaplan[1], Leonard Feldman[3,4], Torgny Gustafsson[3,4] and Manish Chhowalla[1]
*[1]Materials Science and Engineering, [2]Chemistry and Chemical Biology, [3]Physics and Astronomy and [4]Institute of Advanced Materials, Devices and Nanotechnology*

**2:45 Helium Ion Beam Lithography with Novel Sn-Based Photoresist for Extreme Ultraviolet Lithography**
Viacheslav Manichev*[1,3], Mengjun Lia[1,3], Eric Garfunkel[1,3], Leonard C. Feldman[2,3] and Torgny Gustafsson[2,3]
*[1]Chemistry and Chemical Biology, [2]Physics and Astronomy, and Laboratory for Surface Modification and [3]Institute for Advanced Materials Devices and Nanotechnology*

 **3:00 – 3:30 Afternoon Break** 

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## SESSION IV:

## NOVEL APPROACHES

**Chair: Professor Edward W. Castner, Jr.**
**Department of Chemistry and Chemical Biology**

**3:30 Obtaining Thickness-Limited Electrospray Deposition for 3D Coating**
Lin Lei*[1], Dylan A. Kovacevich[1], Michael P. Nitzsche[1], Jihyun Ryu[1], Kutaiba Al-Marzoki[2], Gabriela Rodriguez[3], Lisa C. Klein[2], Andrei Jitianu[3,4] and Jonathan P. Singer[1]
*[1]Mechanical and Aerospace Engineering, [2]Materials Science and Engineering, [3]Chemistry, Lehman College-CUNY and [4]Ph.D. Program in Chemistry and Biochemistry, The Graduate Center of the City University of New York*

**3:45 Surface Impurities on Layered Positive Electrode Materials: Mechanism for Formation and Impact on Performance**
Nicholas Faenza*[1], Lejandro Bruce[1], Zachary W. Lebens-Higgins[2], Irene Plitz[1], Nathalie Pereira[1], Louis F. J. Piper[2] and Glenn G. Amatucci[1]
*[1]Energy Storage Research Group, Materials Science and Engineering and [2] Physics, Applied Physics and Astronomy, Binghamton University*

**4:00 Liquid-Vacuum Interfacial Structure of Ionic Liquids with Fluorinated Anions**
Man Zhao* and Edward W. Castner, Jr.
*Chemistry and Chemical Biology*

**4:15 Surface-Morphology Changes and Damage in Hot Tungsten by Impact to Low-Energy He-Ions**
Hussein Hijazi[1], Céline Martin[2], Pascale Roubin[2], Mark E Bannister[3] and Fred W Meyer[3]
*[1]Physics and Astronomy, [2]Aix-Marseille Université and [3]Oak Ridge National Laboratory*

**4:30 Decoupling the Effects of Surface Topography and Chemistry on the Wetting of Metallic Glasses**
Molla Hasan[1, 3], Juliusz Warzywoda[2] and Golden Kumar[3]
*[1]Mechanical and Aerospace Engineering, [2]Materials Characterization Center, Whitacre College of Engineering, Texas Tech University and [3]Mechanical Engineering, Texas Tech University*

**4:45 Presentation of Theodore E. Madey Student Award: Best Oral Presentation**
**Presentation of Leszek Wielunski Student Award: Best Poster Presentation**

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## ABSTRACTS FOR TALKS

### 9:00 Nearly Triple Point Topological Phase in Half-Metallic GdN

Jinwoong Kim, Heung-Sik Kim and David Vanderbilt
*Physics and Astronomy*

One recently studied topological features is the "triple point" where three bands become degenerate. In contrast to Weyl and Dirac nodes, triple points have nodal lines attached. Here we treat a ferromagnetic material, half-metallic GdN, where the splitting of the triple points depends on the magnetization orientation, enabling a transition between a Weyl-point phase and a "nearly triple point" phase. The nearly triple point phase is revealed to exhibits very similar surface spectra and transport properties compared to a true triple-point system. The rich topological surface states, manipulable via the magnetization orientation, make half-metallic GdN a promising platform for future investigations.

This work was supported by NSF DMR-1629059.

### 9:15 Gapless Magnetic Excitation from Quantum Antiferromagnetic Chains with Strong Spin-Orbit Coupling

Mai Ye*[1], Jae-Wook Kim[1], Choong-Jae Won[2,3], Sang-Wook Cheong[1] and Girsh Blumberg[1]
*[1]Physics and Astronomy, [2]Max Planck POSTECH/Korea Research Initiative, Pohang University of Science and Technology and [3]Laboratory of Pohang Emergent Materials, Pohang Accelerator Laboratory*

We report Raman-scattering and magnetic susceptibility measurements of $Ba_5CuIr_3O_{12}$ single crystals to explore its low-energy magnetic excitation. No magnetic ordering occurs down to 1.8K. We observe a gapless magnetic excitation, peaked at 150cm$^{-1}$ with a FWHM of 200cm$^{-1}$, which has $A_1$ symmetry of $C_{3v}$ group and only appears when the system is excited along the chain direction. The static Raman susceptibility of this magnetic excitation increases from 300K to 50K, but decreases below 50K. The static magnetic susceptibility, on the contrary, increases on cooling below 50K. The low-energy Raman response at 12K obeys a cubic power law, indicating that the quasiparticle dispersion is gapless and linear near the Gamma point. This magnetic excitation probably comes from two-spinon scattering by virtue of strong spin-orbit coupling. Assuming two-spinon scattering, the exchange interaction J is estimated to be about 90cm$^{-1}$ (11meV).

**9:30 The Axion Insulator Phase in Pyrochlore Iridates**

Nicodemos Varnava* and David Vanderbilt
*Physics and Astronomy*

We construct a minimal tight binding model describing pyrochlore iridates. In its magnetic phase, the model exhibits a topological phase in which the Chern-Simons magnetoelectric coupling is quantized to $\pi$ due to the inversion symmetry. This phase is usually referred to as an axion insulator. The rich geometry of the pyrochlore structure enables us to investigate different surface terminations. In the axion phase and when the surface band structure is gapped, we explicitly calculate the anomalous Hall conductivity and show its half-integer quantized nature. Finally, we discuss the factors that decide the sign of this half-quantized response. We find that certain geometries our model predicts, have one-dimensional chiral modes, thus classifying axion insulators as "higher-order" topological insulators.

**9:45 Cluster Dynamical Mean-Field Theory Study of the Deficient Spinel Chalcogenide $GaV_4S_8$**

Heung-Sik Kim, Kristjan Haule and David Vanderbilt
*Physics and Astronomy*

We present a theory of the deficient spinel compound $GaV_4S_8$ (GVS) using a cluster dynamical mean-field (DMFT) approach. GVS has been of growing interest recently because of its multiferroicity below $T_C$~13K. At $T_f$ ~ 70K it has an additional structural transition from a cubic to a rhombohedral structure with cooling. Across the two structural transitions GVS remains insulating with a gap of about ~0.3 eV, and the insulating nature of its high-temperature cubic paramagnetic phase is suspected to be of Mott type. However, there have been no systematic studies of the Mott-insulating phases of GVS, which should be important for understanding the low-temperature ferroelectric and multiferroic phases. To approach this problem, we apply a cluster DMFT method that treats selected atomic orbitals on a cluster of four V atoms, using a molecular orbital basis set instead of an atomic one. Comparing with single-V-site DMFT calculations, we show that intra-cluster correlations are essential in reproducing the Mott-insulating nature of the high-T cubic paramagnetic phase. Correlation effects on the crystal structure of GVS will be also discussed, and the role of Hund's coupling in tuning V clustering by controlling spin-state transitions will be demonstrated.

**10:15 **HIGHLIGHT PRESENTATION****

## The Exciting New Interface Physics

**Ivan Božović**
*Brookhaven National Laboratory*

**(*Oxide*) *Interface Physics.*** The last decade has witnessed explosive growth of research on various oxide heterostructures, and discoveries of exciting new interface phenomena. We may be witnessing the emergence of a new scientific discipline – Interface Physics, delineated by a distinct new set of problems, techniques, phenomena, and theoretical concepts.

***Electronic and/or atomic reconstructions.*** Between the two constituent materials in a heterostructures there is always some mismatch– crystallographic (different lattice constants), electrostatic (violation of local charge neutrality) or dynamic (difference in chemical potentials). The consequences are numerous and profound. The atomic structure can be strained and modified; electronic and/or atomic reconstruction may occur, including large atomic displacements as well as formation of oxygen and/or cation vacancies.

***Metastable structures.*** Most heterostructures are not thermodynamically stable; the synthesis is at least in part kinetically controlled and the atoms are frozen in one out of many nearly-degenerate metastable states. The actual atomic structure at the interface is thus basically impossible to predict. To determine it experimentally, new tools and techniques for study of buried interfaces are required, and being developed fast.

***2D quantum confinement.*** 'Digital' (atomic-layer-by-layer) synthesis yields ultrathin layers with atomically sharp interfaces. Electrons can be extremely confined in one direction, while propagating with high mobility in-plane. Ultrathin metals, superconductors, ferromagnets or ferroelectrics host new phenomena, such as large-scale thermal or quantum critical fluctuations.

***Broken symmetries.*** In any bilayer heterostructure, translational symmetry along the axis perpendicular to the interface is broken, and this can result in large (Rashba) spin-orbit coupling. Other symmetries could be broken as well, resulting in new phenomena such as topological superconductivity.

***Proximity effects.*** Interesting new physics occurs also when the two materials exhibit different order parameters. Competing instabilities, if finely balanced, can result in extreme susceptibility and colossal responses to small perturbations. These may find applications in sensing, ultrafast non-volatile switching, etc., and is hoped to eventually beget new oxide electronics.

In this presentation, a number of simple examples will be given, largely drawn from my own practice with atomic-layer-by-layer molecular beam epitaxy (ALL-MBE) of high-$T_c$ cuprate superconductors [1], but intended to illustrate the more general concepts listed above.

[1] *Nature* **547**, 432 (2017), **536**, 309 (2016), **472**, 458 (2011); **455**, 782 (2008); **422**, 873 (2003); *Science* **326**, 699 (2009); **316**, 425 (2007); **297**, 581 (2002); *Nature Mater.* **12**, 877 (2013); **12**, 387 (2013); **12**, 1019 (2013); **12**, 47 (2013); **11**, 850 (2012); *Nature Phys.* **10**, 256 (2014); **7**, 298 (2011); *Nature Nanotech.* **9**, 443 (2014); **5**, 516 (2010); *Nature Comm.* **2**, 272 (2011); *PRL* **106**, 237003 (2011); **102**, 107004 (2009); **101,** 247004 (2008); **93**, 157002 (2004); **89**, 107001 (2002); *PNAS* **113**, 4284 (2016), **107**, 8103 (2010).

**11:00 Modulation Doping in $LaNiO_3/SrIrO_3$ Superlattices from First Principles**

Michele Kotiuga, Heung-Sik Kim, David Vanderbilt and Karin M. Rabe
*Physics and Astronomy*

High concentration doping, at the level of an electron per formula unit, can stabilize novel phases. Here we study lanthanum nickelate ($LaNiO_3$)/strontium iridate ($SrIrO_3$) superlattices using the first-principles density functional theory (DFT) + U method. Focusing on the 1/1 superlattice, we find that there is a complete modulation doping in which one electron per formula unit is transferred from the $SrIrO_3$ layers to the $LaNiO_3$ layers, resulting in electron-doped nickel layers with valence $Ni^{2+}$ and hole-doped iridium layers with valence $Ir^{5+}$. We will present results on the low energy structures, d-orbital occupations as well as the electronic and magnetic structures.

**11:15 Defect Formation on the Surface of Giant Rashba Systems**

Wenhan Zhang*[1], Damien West[2], Lunyong Zhang[3], Sang-Wook Cheong[1,4], Shengbai Zhang[2] and Weida Wu[1]
*[1]Physics and Astronomy, [2]Physics, Applied Physics and Astronomy, Rensselaer Polytechnic Institute, [3]Laboratory for Pohang Emergent Materials & Max Planck POSTECH Center for Complex Phase Materials, Max Planck POSTECH/Korea Research Initiative, Korea and [4]Rutgers Center for Emergent Materials*

Polar discontinuity at interfaces of different materials may give nontrivial atomic or electronic properties. A well-known case is the interface between insulating $LaAlO_3$ and $SrTiO_3$ perovskites, which possesses electron gas with extremely high carrier mobility [1]. No consensus has been reached regarding the origin of this conductive layer, but many studies indicate polar discontinuity plays a significant role [2,3]. Recently, the family of BiTeX (X= I, Br, Cl) is reported as polar semiconductors with giant Rashba-type spin splitting effect [4,5]. They have drawn intensive research interests since then because of the great potentials for practical spintronic functions. The bulk polar atomic corrugations give rise to significant polar discontinuities near the surface. Via scanning tunneling microscopy (STM), we found that the cleaving temperature can dramatically influence the defect formation on the surface of giant Rashba semiconductor BiTeCl. Here, we will present the detailed STM and DFT studies to understand the underlying mechanism.

[1] A. Ohtomo, and H. Y. Hwang. Nature 427.6973 (2004).
[2] M. Huijben *et al.* Nat. Mater. 5, 556 (2006).
[3] M. S. Park *et al.* Phys. Rev. B 74, 205416 (2006).
[4] K. Ishizaka *et al.* Nat. Mater. 10, 521 (2011).
[5] S. V. Eremeev *et al.* Phys. Rev. Lett. 108, 246802 (2012).

**11:30 Current-Density Implementation for Calculating Flexoelectric Coefficients**

Cyrus E. Dreyer[1], Massimiliano Stengel[2,3] and David Vanderbilt[1]
*[1]Physics and Astronomy, [2]ICREA-Institució Catalana de Recerca i Estudis Avançats, Barcelona, Spain and Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Campus UAB, Bellaterra, Spain*

The flexoelectric (FxE) effect, where polarization is induced by a strain gradient, is universal in all insulators. As devices shrink to the micro and nano scale, large strain gradients can occur, and therefore the FxE effect can play a significant role in their electrical and mechanical properties; also, the FxE effect can be exploited for novel device design paradigms such as piezoelectric ``meta-materials" constructed from nonpiezoelectric constituents, or mechanical switching of ferroelectric polarization. One of the crucial limitations to understanding and exploiting the FxE effect is the lack of an efficient first-principles methodology to calculate all of the components of the bulk FxE tensor; the transverse and shear components in particular are problematic. In this work we develop such a methodology based on density functional theory to calculate the full bulk, clamped-ion FxE tensor from a single unit cell by calculating the current-density response to the adiabatic displacement of atoms from a long wavelength acoustic phonon. We benchmark our methodology on simple systems of isolated nobel gas atoms, and apply it to calculate the clamped-ion flexoelectric constants for a variety of technologically important cubic materials.

**11:45 An Unusual Example of Kinetically-Trapped Molecular Self-Assembly: ZnTPP on Ag(100)**

Sylvie Rangan[1], Peter Kim[1], Charles Ruggieri[1], Robert A. Bartynski[1] and Steven Whitelam[2]
*[1]Physics and Astronomy and Laboratory for Surface Modification and [2]Molecular Foundry, Lawrence Berkeley National Laboratory*

The result of the self-assembly of organic molecules on a noble metal surface is often analyzed in terms of equilibrium configurations, implicitly assuming that molecular adsorbates are mobile enough to reach global thermodynamic equilibrium. For example, tetraphenylporphyrins (TTPs), which have a square symmetry and a high surface mobility, generally assemble on surfaces in a highly-ordered square array, locked in-place by phenyl T-stacking. Here, using scanning tunnel microscopy, a highly ordered metastable [2+1] phase is observed for a monolayer of ZnTPP molecules self-assembled at 300K on Ag(100). The usually reported [1+1] square phase is found only after higher temperature anneal. Using a Kinetic Monte Carlo model, molecular self-assembly is simulated and reveals that this system is an unusual example of 2D molecular growth, where kinetic factors are the limiting process directing self-assembly.

**1:00** **<u>HIGHLIGHT PRESENTATION</u>****

### 2D Materials: Surfaces, Interfaces and Defects

**<u>Robert M. Wallace</u>**
*Materials Science and Engineering, The University of Texas at Dallas*

The size reduction and economics of integrated circuits, captured since the 1960's in the form of Moore's Law, is under serious challenge. Current industry roadmaps reveal that physical limitations include reaching aspects associated with truly atomic dimensions, and the cost of manufacturing is increasing such that only 2 or 3 companies can afford leading edge capabilities. To address some of the materials physical limitations, "2D materials" such as graphene, phosphorene, h-BN, and transition metal dichalcogenides have captured the imagination of the electronics research community for advanced applications in nanoelectronics and optoelectronics. Among 2D materials "beyond graphene," some exhibit semiconducting behavior, such as transition-metal dichalcogenides (TMDs), and present useful bandgap properties for applications even at the single atomic layer level. Examples include "MX2", where M = Mo, W, Sn, Hf, Zr and X = S, Se and Te.

In addition to the potentially useful bandgaps at the monolayer thickness scale, the atomically thin layers should enable thorough electric field penetration through the channel, thus enabling superior electrostatic control. Further, with such thin layers, the integration with suitable gate dielectrics can result in a mobility enhancement. From an interface perspective, the ideal TMD channel material should have a dearth of dangling bonds on the surface/interface, resulting in low interface state densities, which are essential for efficient carrier transport. The ideal TMD materials have much appeal, but the reality of significant densities of defects and impurities will surely compromise the intrinsic performance of such device technologies. This presentation will examine the state-of-the-art of these materials in view of our research on semiconductor device applications, and the challenges and opportunities they present for electronic and optoelectronic applications. [1]

[1] S. J. McDonnell and R.M.Wallace, *Thin Solid Films*, **616**, 482-501 (2016).

**1:45** **Chemical Vapor Deposition Growth of Metallic Niobium Disulfide**

<u>Xiuju Song</u>, Yan Wangand and Manish Chhowalla
*Materials Science and Engineering*

Two-dimensional metallic niobium disulfide ($NbS_2$) is attracting much attention. It is a promising catalyst for hydrogen evolution reaction (HER), as well as an ideal electrode for the semiconducting TMD materials. However, the synthesis of such interesting $NbS_2$ material with controllable thickness in large scale is a big challenge. Herein, we fabricate thickness-tunable $NbS_2$ flakes and centimeter-sized films via a chemical vapor deposition (CVD) method. The grown $NbS_2$ flakes are mixed 3R and 2H phases according to the Raman spectra, XPS spectra and TEM results. The electric measurement demonstrates the metallic property of the CVD-grown $NbS_2$ flakes.

**2:00 Indium Contacts for Minimizing Contact Resistance of 2D $MoS_2$ Field Effect Transistors**

Yan Wang *[1], Jieun Yang[1], Xiuju Song[1,2], Fang Zhao[3] and Manish Chhowalla[1]
*[1]Materials Science and Engineering, [2]College of Optoelectronic Engineering, Shenzhen University and [3]Physics, Princeton University*

A major challenge in achieving high-performance field effect transistors (FETs) with two-dimensional molybdenum disulfide is the minimization of contact resistance between the semiconducting material and the metal electrode. Different approaches such as phase engineering[1], doping of source and drain electrodes[2] and interface de-pinning[3] to reduce contact resistance have been studied. Here, we present a systematic study of high-performance few layered $MoS_2$ FETs with indium as electrodes. FET devices using In contacts consistently exhibit substantially better performance in terms of the on/off ratio, mobility and drive currents. The contact resistance we obtained using transfer length method is 1.8 $k\Omega \cdot \mu m$.

1. Kappera, R. et al. Phase-engineered low-resistance contacts for ultrathin MoS2 transistors. Nat. Mater. **13,** 1128–1134 (2014).
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3. Kaushik, N., Karmakar, D., Nipane, A., Karande, S. & Lodha, S. Interfacial n-Doping Using an Ultrathin TiO2 Layer for Contact Resistance Reduction in MoS2. ACS Appl. Mater. Interfaces **8,** 256–263 (2016).

**2:15 Stripe Quadrupole Order in the Nematic Phase of FeSe**

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Superconductivity in the iron-based superconductors (FeSCs) often occurs in close proximity to electronic nematic state in which the four-fold rotational symmetry is broken. For most of the FeSCs, the nematic phase transition is closely followed by the magnetic phase transition, leading to a persistent controversy about the essential relevance of spin and charge orders to superconductivity. Using the polarization-resolved electronic Raman spectroscopy, we report the observation an unexpected gap in the orthorhombic phase of the non-magnetic $FeSe_{1-x}S_x$ superconductor, which is interpreted as formation of a stripe-type charge quadrupole order. The discovery of the hidden quadrupole order naturally explains the recently reported puzzling orbital selective superconductivity in FeSe, as well as the enhanced superconducting transition temperature in monolayer FeSe films.

**2:30 Correlation of Atomic Scale Defects Using He Ion Beam in 2D $MoS_2$ with Optical, Electronic and Catalytic Properties**

Jieun Yang*[1], Slava Manichev[2,4], Maureen Lagos[1,4], Raymond Fullon[1], Yan Wang[1], Xiuju Song[1], Ibrahim Bozkurt[1], Daniel Kaplan[1], Leonard Feldman[3,4], Torgny Gustafsson[3,4] and Manish Chhowalla[1]
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Defects can strongly influence the electrical, optical, and chemical properties of materials. For example, it is now well known that while the basal plane of 2H-$MoS_2$ is typically chemically inert, it can be made active for hydrogen evolution reaction (HER) by introducing defects in the form of sulfur vacancies. Furthermore, properties of $MoS_2$ can be tuned from semiconducting to metallic to insulating by controlling the defect concentration. However, understanding defect-induced changes in properties at the atomic scale remains a challenge. In this study, we have used the helium ion beam microscope (HIM) to rationally induce atomic scale defects and control their concentrations within the channels of pre-patterned field effect transistors (FETs). We have then characterized the nature of the atomic defects (S vacancies, Mo vacancies) in the scanning transmission electron microscope (STEM). In addition, we have measure the Raman spectra and photoluminescence along with transport in the FET configuration. We are thus able to correlate how the type and number of defects influence PL and mobility in thin $MoS_2$. We found that the properties degenerate with defects, as expected, but there is a transition from semiconducting to metallic behavior at defect concentrations above 20%. Additionally, we were able to correlate HER activity of $MoS_2$-based catalysts with defect concentration and electrical properties.

**2:45 Helium Ion Beam Lithography with Novel Sn-Based Photoresist for Extreme Ultraviolet Lithography**

Viacheslav Manichev*[1,3], Mengjun Lia[1,3], Eric Garfunkel[1,3], Leonard C. Feldman[2,3] and Torgny Gustafsson[2,3]
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As Helium Ion Microscopy matures, more applications are emerging taking advantage of its unique properties. The sub-nanosized He beam has two orders of magnitude increased sensitivity for most photoresists when compared to an e-beam. Here we demonstrate the use of a novel organo-tin photoresist for extreme ultraviolet (~ 93 eV) lithography. β-$NaSn_{13}([NaO_4(BuSn)_{12}(OH)_3(O)_9(OCH_3)_{12}(Sn(H_2O)_2)])$ is a cluster that uses tin for its high atomic photon absorption cross section, a central factor that determines the optimal elements around which to base photoresist chemistry. The 0.3 nm He ion beam is capable of producing high aspect ratio features (15:1) and dense line patterns with 20 nm half pitch. Even smaller features were generated by thinning the photoresist layer prior to exposure. Also, the dose and substrate dependence was investigated.

*This work was supported by Rutgers Institute for Advanced Materials, Devices and Nanotechnology and performed in collaboration with May Nyman et al. at Oregon State University with funding from the NSF-Center for Chemical Innovation under Grant CHE-1606982.*

**3:30 Obtaining Thickness-Limited Electrospray Deposition for 3D Coating**

Lin Lei*[1], Dylan A. Kovacevich[1], Michael P. Nitzsche[1], Jihyun Ryu[1], Kutaiba Al-Marzoki[2], Gabriela Rodriguez[3], Lisa C. Klein[2], Andrei Jitianu[3,4] and Jonathan P. Singer[1]
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The electrospray process utilizes the balance of electrostatic forces and surface tension within a charged spray to produce charged microdroplets with a narrow dispersion in size. In electrospray deposition, each droplet carries a small quantity of suspended material to a target substrate. A self-limited spray, has only been observed in the spray of insulating materials onto conductive substrates. In such sprays, a limiting thickness emerges where the accumulation of charge repels further spray. In this study, we examined the parametric spray of several glassy polymers by adjusting critical parameters for thickness-limited sprays. The key parameters for determining the limiting thickness were field strength and the spray temperature. Moreover, these control mechanisms can be applied to the uniform or controllably varied microscale coating of complex 3D objects.

**3:45 Surface Impurities on Layered Positive Electrode Materials: Mechanism for Formation and Impact on Performance**

Nicholas Faenza*[1], Lejandro Bruce[1], Zachary W. Lebens-Higgins[2], Irene Plitz[1], Nathalie Pereira[1], Louis F. J. Piper[2] and Glenn G. Amatucci[1]
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Enhancing the functionality of layered, R-3m positive electrode materials for lithium-ion batteries is dependent on a comprehensive understanding of the failure modes prevalent in state of the art batteries. While it is well known that layered oxide materials are unstable in ambient air and form various surface impurities, the specific reaction sequences that develop $Li_2CO_3$ and other species remain unclear. A unique combination of atmospheric exposure and thermal treatments enabled the isolation and characterization of individual surface species that developed on $LiNi_{0.8}Co_{0.15}Al_{0.05}O_2$. The impact of each impurity specie on the host material's electrochemical performance was thoroughly analyzed, and the degradation reaction mechanisms are proposed.

**4:00 Liquid-Vacuum Interfacial Structure of Ionic Liquids with Fluorinated Anions**

Man Zhao* and Edward W. Castner, Jr.
*Chemistry and Chemical Biology*

Ionic liquids (ILs) are salts that have low melting points, usually below room temperature. They are composed of cations and anions. Ionic liquids display sponge-like heterogeneous bulk structures due to the coexistence of polar domains and nonpolar domains. The structure of ionic liquids is significantly influenced by confinement and by interactions with interfaces. When put in vacuum, the structure of ionic liquids with long alkyl tails on both cations and anions will transform from sponge-like structure to lamellar-like. In this work, molecular dynamic (MD) simulations are carried out for several ionic liquids with 1-octyl-3-methylimidazolium ($Im_{1,8}^{+}$) cations and fluorinated anions. The densities along the z-axis are obtained to analyze the structures at interface.

**4:15 Surface-Morphology Changes and Damage in Hot Tungsten by Impact to Low-Energy He-Ions**

Hussein Hijazi[1], Céline Martin[2], Pascale Roubin[2], Mark E Bannister[3] and Fred W Meyer[3]
[1]*Physics and Astronomy,* [2]*Aix-Marseille Université and* [3]*Oak Ridge National Laboratory*

Due to several favorable physical properties, tungsten is chosen as the plasma facing material for magnetic fusion devices such as ITER. During the deuterium-tritium fusion operation of ITER, significant helium ash will be formed and its interaction with tungsten wall materials is currently undergoing extensive evaluation. In this contribution, we report results of measurements on the evolution of the surface morphology of a hot tungsten surface due to impact by He ions, performed at the ORNL Multicharged Ion Research Facility. Surface-morphology changes were investigated over a broad range of fluences, energies and temperatures. At low fluences, ordered coral- and ridge-like surface structures are observed, with great grain-to-grain variability. At the largest fluences, individual grain characteristics disappear in FIB/SEM scans, and the entire surface is covered by a multitude of near-surface bubbles, and disordered whisker growth. Different scenarios for the whisker growth will be presented.

**4:30 Decoupling the Effects of Surface Topography and Chemistry on the Wetting of Metallic Glasses**

Molla Hasan[1, 3], Juliusz Warzywoda[2] and Golden Kumar[3]
*[1]Mechanical and Aerospace Engineering, [2]Materials Characterization Center, Whitacre College of Engineering, Texas Tech University and [3]Mechanical Engineering, Texas Tech University*

We report the effects of surface patterning on the wetting of $Pt_{57.5}Cu_{14.7}Ni_{5.3}P_{22.5}$ and $Pd_{43}Cu_{27}Ni_{10}P_{20}$ metallic glasses. To maintain the integrity of surface chemistry of the metallic glasses, we optimize thermoplastic patterning protocol and use chemical-free demolding. Our results show that single-scale surface microstructures can render inherently hydrophilic $Pt_{57.5}Cu_{14.7}Ni_{5.3}P_{22.5}$ metallic glass hydrophobic when its chemical state is preserved. We also observe that because of oxidation, $Pd_{43}Cu_{27}Ni_{10}P_{20}$ metallic glass remains hydrophilic regardless of its surface topography, though its wettability evolves (i.e. decreases) with time due to airborne contamination. These results suggest that to draw an unambiguous conclusion about the role of surface topography, concomitant changes in surface chemistry must be avoided.

# THIRTY-SECOND ANNUAL SYMPOSIUM
# LABORATORY FOR SURFACE MODIFICATION/ INSTITUTE FOR ADVANCED MATERIALS, DEVICES AND NANOTECHNOLOGY

## ABSTRACTS FOR POSTERS

### 1) Characterization of Highly Active Electrodeposited $Li_xCoO_2$ Thin Films for Enhanced OER in PGM-Free Photoelectrochemical Cells

Ajay Kashi*[1], Shinjae Hwang[2], Anders B. Laursen[2] and G. Charles Dismukes[2]
*[1]Chemical and Biochemical Engineering and [2]Chemistry and Chemical Biology*

In the development of high-performance, commercially-scalable photoelectrochemical cells (PECs) for solar-driven hydrogen production, effective and low-cost anodes must be engineered for long-term operation in alkaline solution. Lithium cobalt oxide (LiCoO2) has been studied as a highly active and stable catalyst for the anodic oxygen evolution reaction (OER) in its cubic spinel polymorph, LiCo2O4.

In this study, thin films of LixCoO2 have been electrodeposited onto a Ti/TiOx support for functional integration as the dark anode in the PEC device. Kinetic performance as evaluated by cyclic and linear sweep voltammetry resulted in geometric current densities of 10 mA/cm2 (corresponding to 10% photoelectrochemical conversion) achieved at 430 mV overpotential. Long-term stability measurements evaluated at 10 mA/cm2 demonstrate continuous operation for up to 13 days with minimal loss in activity.

### 2) Observation of Resonances in the Raman Cross Section of Surface Phonons in on $Bi_2Se_3$, $Bi_2Te_2Se$ and $Bi_2Te_3$

A. -C. Lee*[1], H.-H Kung[1], S. -W. Cheong[1], R. Merlin[2], I. Boulares[2] and Girsh Blumberg[1,3]
*[1]Physics & Astronomy, [2]Physics, University of Michigan and [3]National Institute of Chemical Physics and Biophysics, Estonia*

The dynamics of electron-phonon coupling at the surface of a TI has been shown to behave differently than in the bulk. The Raman cross section as a function of excitation energy provides information about resonance conditions for inter-band transitions, and can be used to determine the optimal excitation energy for observing surface and bulk related phenomena simultaneously. Here, we present the results of Raman scattering experiments on $Bi_2Se_3$, $Bi_2Te_2Se$, and $Bi_2Te_3$ single crystals, which show both bulk and surface related features in the low energy regime (< 200$cm^{-1}$). Both the bulk and surface features are resonant at the same energy, indicating the resonance condition in both systems share the same physical origin.

**3) Availability of the Elements for Heterogeneous Catalysis – Predicting the Industrial Viability of Novel R&D Catalysts**

Anders B. Laursen[1,2], Jens Sehested[3], Ib Chorkendorff[2] and Peter C. K. Vesborg[2]
*[1]Chemistry and Chemical Biology, [2]Physics at Technical University of Denmark and [3]Haldor Topsoe A/S*

Concerns the chemical industry's sustainability drives the development of more efficient catalytic reactions. 1st-generation estimates of catalyst viability based on crustal abundance poses severe limitations. Here, we develop a 2nd-generation guiding principle for predicting the viability of novel catalysts to impact the global chemical industry. We describe a correlation between catalyst consumption and element production/price, for 11 representative industrial catalytic processes. Based on this correlation, we introduce two new descriptors for the catalyst viability allowing the identification of general limits of viability. We extend this analysis to calculate the predicted limits of economic viable production and product cost for novel catalysts.

**4) Thermocapillary Multidewetting of Thin Films**

Arielle Marie Gamboa*, Michael Nitzsche, Valeria Saro-Cortes, Tianxing Ma, Lin Lei and Jonathan Singer
*Mechanical and Aerospace Engineering*

Thermocapillary dewetting of liquids and molten films has recently emerged as a viable alternative to conventional microprocessing methods. Its dependence on thermal gradients allows it to be applied to various combinations of materials, including metals and polymers, with sufficiently different melting points. By subjecting these molten films to concentrated laser spots, materials can be individually patterned, providing an avenue to create aligned morphologies. Among these novel patterns are arrays of concentric holes, lines with periodic segmentation, or directed growths on holes. Various factors can be manipulated to control features, ranging from spot size, temperature, film thickness, and exposure time.

**5) Topographical Constraints on the Permeation of Electrosprayed Particles**

Dylan Kovacevich*, Lin Lei and Jonathan P. Singer
*Mechanical and Aerospace Engineering*

Our previous work established that electrospray deposition can be used to conformally coat complex 3D surfaces in non-conductive material through a self-limiting effect. In this process, the Coulombic repulsion of sprayed particles from an already coated surface prevents additional material from being deposited. When applied in 3D, the interiors of features such as pores and channels may receive reduced coverage. By hexagonally packing ball bearings of varying diameter to create a network of narrow pathways, we establish the limits of this process.

**6) Spatially Resolved High-Resolution Core Shell Electron Energy Loss Studies of Interfaces in Semiconductor Devices**

Hongbin Yang*[1], Eric L. Garfunkel[1] and Philip E. Batson[2,3]
*[1]Chemistry and Chemical Biology, [2]Physics and Astronomy and [3]Materials Science and Engineering*

Developing an atomic scale understanding of interfaces in semiconductor devices is a necessary precursor to rationally design materials and processing routes to improve device performance. Here we study the interface of silicon with several metal oxides and nitrides using the Rutgers Nion UltraSTEM. With its extraordinary energy resolution, we obtain spatially resolved high-resolution core shell electron energy loss spectra for silicon, oxygen and nitrogen. We correlate the conduction band structure with our spectra as a way to understand the bonding and electronic structure at the interfaces.

**7) Solution to the Hole-Doping Problem and Tunable Quantum Hall Effect in $Bi_2Se_3$ Thin Films**

Jisoo Moon*[1], Nikesh Koirala[1], Maryam Salehi[2], Wenhan Zhang[1], Weida Wu[1] and Seongshik Oh[1]
[1]*Physics and Astronomy and* [2]*Materials Science and Engineering*

$Bi_2Se_3$, one of the most widely studied topological insulators (TIs), is naturally electron-doped due to n-type native defects. However, many years of efforts to achieve p-type $Bi_2Se_3$ thin films have failed so far. In this presentation, we provide a solution to this long-standing problem, showing that the main culprit has been the high density of interfacial defects. By suppressing these defects through an interfacial engineering scheme, we have successfully implemented p-type $Bi_2Se_3$ thin films down to the thinnest topological regime. On this platform, we present the first tunable quantum Hall effect (QHE) study in $Bi_2Se_3$ thin films, and reveal not only significantly asymmetric QHE signatures across the Dirac point but also the presence of competing anomalous states near the zeroth Landau level.

**8) Perovskite-Based Oxyhydrides as Potential Ammonia Catalysts**

Joshua Flynn, Martha Greenblatt and Gerard Dismukes
*Chemistry and Chemical Biology*

Ammonia ($NH_3$) is in high global demand as it is essential for fertilizers. Current industrial $NH_3$ production is based on the 100-year-old Haber-Bosch method which has proven to be effective for mass production of $NH_3$ from dinitrogen ($N_2$) and dihydrogen ($H_2$) gas but is extremely energy intensive requires high operating temperatures (>500 °C) and pressures (>150 atm) to break the strong triple bond in $N_2$. A new class solid state perovskite-type oxyhydrides have recently emerged and $BaTiO_{3-x}H_x$ is reported to undergo $N^{3-}/H^-$ exchange by heating under $N_2$. This indicates that the exchange can break the $N_2$ triple bond and presents the opportunity to study these materials as potential $N_2$ reduction catalysts.

**9) Selective Electrochemical $CO_2$ Reduction to C3 and C4 Carbohydrates Exceeding 90% Energy Efficiency**

Karin U. D. Calvinhoa*, Anders B. Laursena, Kyra M. K. Yapa, Krishani Teeluck and G. Charles Dismukes
*Chemistry and Chemical Biology*

Electrochemical carbon dioxide reduction reaction ($CO_2RR$) is a promising way to recycle $CO_2$ into fine chemicals that are currently derived from fossil fuels. Here we introduce nickel phosphides as a novel catalyst family for $CO_2RR$, with high selectivity to C3 (methylglyoxal) and C4 (2,3-furandiol) products at overpotentials as low as 10 mV. We have proposed a scheme for the formation of multi-carbon products where hydride transfer enables the reduction of $CO_2$ at near zero overpotentials. This reaction paradigm, previously unseen in heterogeneous catalysts, opens a novel energy-efficient mechanism for the synthesis of valuable chemicals.

**10) Mechanistic Studies on Nickel Phosphide Electrocatalysts for the Carbon Dioxide Reduction Reaction**

Krishani M. Teeluck*, Karin U. D. Calvinho, Anders B. Laursen and G. Charles Dismukes
*Chemistry and Chemical Biology*

The electrochemical carbon dioxide reduction reaction ($CO_2RR$), used to convert $CO_2$ to useful chemicals, is a convenient solution to its saturation levels in our atmosphere, while creating a carbon-neutral cycle based entirely on renewable resources. Ni2P is the first catalyst shown to produce a valuable $C_4$ product at only 10 mV overpotential and with 71% selectivity. However, the reaction mechanism is still largely unknown, presenting a critical problem for optimizing these electrocatalysts. We therefore explored the $CO_2RR$ mechanism by reducing possible intermediates in lieu of $CO_2$. We found that that formic acid and methylglyoxal are intermediates in this reaction, leading to the formation of 2,3-furandiol through aldol condensation.

**11) Titanium Nitride as a Conducting Interfacial Layer Between Hydrogen Evolution Catalysts and Silicon Photocathodes for Stable Solar-to-Hydrogen Water Splitting Devices**

Shinjae Hwang*, Spencer H. Porter, Anders B. Laursen, Hongbin Yang, Mengjun Li, Viacheslav Manichev, Karin Calvinho, Voshadhi Amarasinghe, Martha Greenblatt, Eric Garfunkel and G. Charles Dismukes
*Chemistry and Chemical Biology*

The development of highly efficient photoelectrochemical cells (PECs) that can split water into $H_2$ and $O_2$ is a grand challenge in the field of renewable energy. Low-cost, efficient electrocatalysts using transition metal phosphides (TMP) for hydrogen evolution have been developed, but few reports have demonstrated their successful integration with a photoabsorber owing to unstable junction formation. To prepare a monolithic junction, a catalyst/diffusion barrier/photoabsorber stack consisting of $NiP_2$, TiN, and $n^+$p-Si made up the photocathode reported herein. The photocathode produces similar $J_{sc}$ compared to bare Si, and maintains a stable hydrogen evolution photocurrent (±10%) without failure

for at least 125 hours in acid (0.5 M $H_2SO_4$), the duration of testing. Supported by the NSF-CBET/DOE-EERE.

**12) Measuring the Surface Damage of Femtosecond Pulse Radiation by Channeling RBS**

Ryan Thorpe[1], Andrey Baydin[2], Halina Krzyzanowska[2], Thomas Schenkel[3], Norman Tolk[2], Leonard Feldman[1] and Torgny Gustafsson[1]
*[1]Physics and Astronomy and Laboratory for Surface Modification, [2]Vanderbilt University, Nashville, TN and [3]Lawrence Berkeley National Lab, Berkeley, CA*

An active area of research in radiation physics is the interaction of ultra-fast ion pules with solids and the subsequent non-linear effects. The BELLA petawatt laser at LBNL has the ability to deliver 30 fs, 40 J pulses to a target. By focusing these pulses on a thin Ti foil, an energetic multi-ion beam is formed from the vaporized Ti, as well as H, C, and O from water and carbonaceous species on the surface of the foil. Of particular interest is the residual crystal damage associated with such a radiation source, whose proton energies range up to 6 MeV. Defect kinetics, defect annihilation, and unique thermal effects are all expected to be modified compared to DC beams. In the final analysis one might seek new, metastable materials as the activation energies for the individual processes are modified.

Using channeling RBS at the Rutgers 1.7 MeV Tandetron, we are characterizing the implanted species arising from the BELLA source as well as the surface damage on semiconductor crystals. Initial results revealed an unexpected accumulation of Ti metal clusters on the sample surface, with possible indications of Ti penetration into the solid. This work paves the way for future comparisons between pulsed beam radiation damage and DC beam damage.

**13) Rubrene vs Fluorine-Functionalized Rubrene Molecules: Self-Assembly, Electronic Structure and Energy Alignment**

Jonathan Viereck*, Sylvie Rangan and Robert A. Bartynski
*Physics and Astronomy and Laboratory for Surface Modification*

The influence of fluorine-functionalization of the rubrene molecule is explored by comparing rubrene and a fluorinated rubrene (FM-rubrene), adsorbed on a Ag(100) surface. The self-assembly, studied using scanning tunneling microscopy, reveals highly ordered molecular assemblies at the monolayer level, that are incompatible with epitaxial growth of rubrene or FM-rubrene ordered crystals. Moreover, the molecular order has a direct influence on the resulting electronic structure and energy alignment of the molecular levels with the band edges of Ag(100), measured using UV and inverse photoemission spectroscopies. A careful comparison of the adsorption of rubrene and FM-rubrene on Ag(100) enables a fundamental understanding of the molecular-surface and inter-molecular interactions, as well as their effects on molecular crystal growth and energy alignment with supporting surfaces.