

RPPR Final Report

as of 17-Sep-2018

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INVESTIGATOR(S):

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Final Report for Period Beginning 03-Apr-2018 and Ending 02-Sep-2018

Title: 2018 Materials Research Society (MRS) Spring Meeting

Begin Performance Period: 03-Apr-2018

End Performance Period: 02-Sep-2018

Report Term: 0-Other

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Distribution Statement: 1-Approved for public release; distribution is unlimited.

STEM Degrees: 0

STEM Participants: 0

Major Goals: The MRS meeting is the world's foremost international scientific gathering for materials research that showcases leading interdisciplinary research in both fundamental and applied areas and is coordinated by over 200 scientists from both academia and industry in many countries around the world. The Army Research Office grant enabled the symposia organizers to provide travel reimbursements for invited speakers, early career researchers and students to participate in the meeting. It also provided students and postdocs the opportunity to network with preeminent senior researchers both domestic and international.

Symposia receiving Army Research Office support are:

Symposium EN15, Novel Materials Physics of Perovskite Semiconductors

Symposium EP06, Materials, Devices and Systems for Machine Learning and Neuromorphic Computing

Symposium NM11, Deformable Atomically-Thin Materials -- Mechanics, Materials and Devices

Accomplishments: Symposium EN15: The quick growth of research on lead halide perovskites in the past several years not only offers an interesting class of materials for photovoltaic application, but it also demonstrates high defect tolerance in these materials. Understanding the mechanisms behind the defect tolerance and transplanting the mechanisms to other stable perovskite semiconductors would potentially lead to a transformative leap in semiconductor research. This symposium was dedicated to dissemination and discussion of novel materials physics of perovskite semiconductors.

Symposium EP06: The goal was to provide an overview of current active topics of research in materials science targeted at developing new materials for analytics and neuromorphic computing. It featured invited talks from researchers who provided high-level views of machine learning trends, requirements from systems development perspectives, as well as cutting-edge developments in new materials systems such as memristors, chalcogenides, magnetic and ferroelectric materials. It brought together researchers who are developing new materials and novel nanoscale device structures aimed to design a new generation of information processing engines that are not limited by the constraints of conventional (von Neumann) architecture.

Symposium NM11: This symposium covered fundamental mechanics theory and modeling of atomically-thin materials and devices, elucidating how controlled deformation and strain engineering can enable new materials properties and device functions. On the experimental side, it covered advances in material synthesis and assembly/processing as well as controlled deformation and straining of atomically-thin materials. Interdisciplinary topics related to mechanics, physics, and materials science and engineering were presented by invited speakers in order to accelerate the development of new forms of materials and applications. The presentations were also

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aimed to motivate synergistic research collaboration in the field of deformed and strained atomically-thin materials.

Training Opportunities: Nothing to Report

Results Dissemination: 2018 MRS Spring Meeting program and abstracts are posted to the MRS website: www.mrs.org

Papers that have been submitted and approved are published in MRS Advances (e-Proceedings): <https://www.cambridge.org/core/journals/mrs-advances>

Honors and Awards: Nothing to Report

Protocol Activity Status:

Technology Transfer: Nothing to Report

PARTICIPANTS:

Participant Type: Other Professional

Participant: Yi-Yan Sun PhD

Person Months Worked: 1.00

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Funding Support:

Participant Type: Other Professional

Participant: Bipin Rajendran PhD

Person Months Worked: 1.00

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Funding Support:

Participant Type: Other Professional

Participant: SungWoo Nam PhD

Person Months Worked: 1.00

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Funding Support:

ARTICLES:

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Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published

Journal: MRS Advances

Publication Identifier Type: DOI

Publication Identifier: 10.1557/adv.2018.460

Volume: Issue:

First Page #: 1

Date Submitted: 7/20/18 12:00AM

Date Published: 5/1/18 4:00AM

Publication Location: Warrendale PA

Article Title: Crystal Lattice Dynamics of the Substitutional Solid Solutions in the Bi(Gd) - Fe - O and Bi(Nd) - Fe - O Systems

Authors: Valery Sobol, Barys Korzun, Cheslav Fedorcov, Olga Mazurenko, Temirkhan Bizhigitov, Sabit Tomaev,

Keywords: chemical substitution x-ray diffractin (XRD) infrared (IR) spectroscopy

Abstract: The substitutional solid solutions in the Bi(Gd) - Fe - O and Bi(Nd) - Fe - O systems of the Bi_{1-x}GdxFeO₃ and Bi_{1-x}NdxFeO₃ types with x up to 0.20 were synthesized by the solid-state reaction method and investigated using X-ray diffraction analysis and infrared reflective spectrometry in the wavelength range from 12.5 to 24 μm. It was determined that the Bi_{1-x}GdxFeO₃ and Bi_{1-x}NdxFeO₃ crystal structure is a distorted form of perovskite, R3c space group. Two extremums at 18.2 μm (strong extremum) and 22.5 μm (rather weak extremum) on the infrared reflection spectra of the Bi_{1-x}GdxFeO₃ and Bi_{1-x}NdxFeO₃ solid solutions were discovered. The extremum at 18.2 μm corresponds to the Fe - O stretching vibrations and the extremum at 22.5 μm corresponds to the O - Fe - O bending vibrations of the FeO₆ groups.

Distribution Statement: 1-Approved for public release; distribution is unlimited.

Acknowledged Federal Support: **N**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published

Journal: MRS Advances

Publication Identifier Type: DOI

Publication Identifier: 10.1557/adv.2018.497

Volume: Issue:

First Page #: 1

Date Submitted: 7/20/18 12:00AM

Date Published: 6/1/18 4:00AM

Publication Location: Warrendale PA

Article Title: The effect of an improved density functional on the thermodynamics and adsorption-controlled growth windows of chalcogenide perovskites

Authors: Stephen A. Filippone, Yi-Yang Sun, R. Jaramillo

Keywords: thermodynamics molecular beam epitaxy (MBE) perovskites physical vapor desposition (PVD) phase equilibria

Abstract: Ternary sulfides and selenides in the distorted-perovskite structure ("chalcogenide perovskites") are predicted by theory to be semiconductors with band gap in the visible-to-infrared and may be useful for optical, electronic, and energy conversion technologies. Density functional theory can be used in combination with computational thermodynamics to predict the pressure-temperature phase diagrams for chalcogenide perovskites. We report results using the Strongly Constrained and Appropriately Normed (SCAN) and the rVV10 density functionals, and compare to previously-published results using the PBEsol functional. We highlight the windows of thermodynamic equilibrium between solid chalcogenide perovskites and the vapor phase at high temperature and very low pressure. These phase diagrams can guide adsorption-limited growth of ternary chalcogenides by molecular beam epitaxy (MBE).

Distribution Statement: 1-Approved for public release; distribution is unlimited.

Acknowledged Federal Support: **N**

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Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published

Journal: MRS Advances

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Publication Identifier: 10.1557/adv.2018.413

Volume: Issue:

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Date Submitted: 7/20/18 12:00AM

Date Published: 4/1/18 4:00AM

Publication Location: Warrendale PA

Article Title: Enhanced Grain Size and Crystallinity in CH₃NH₃PbI₃ Perovskite Films by Metal Additives to the Single-Step Solution Fabrication Process

Authors: Zahrah S. Almutawah, Suneth C. Watthage, Zhaoning Song, Ramez H. Ahangharnejhad, Kamala K. Su

Keywords: perovskites Cd crystalline grain size Zn

Abstract: Methods of obtaining large grain size and high crystallinity in absorber materials play an important role in fabrication of high-performance methylammonium lead iodide (MAPbI₃) perovskite solar cells. Here we study the effect of adding small concentrations of Cd²⁺, Zn²⁺, and Fe²⁺ salts to the perovskite precursor solution used in the single-step solution fabrication process. Enhanced grain size and crystallinity in MAPbI₃ films were obtained by using 0.1% of Cd²⁺ or Zn²⁺ in the precursor solution. Consequently, solar cells constructed with Cd- and Zn-doped perovskite films show a significant improvement in device performance. These results suggest that the process may be an effective and facile method to fabricate high-efficiency perovskite photovoltaic devices.

Distribution Statement: 1-Approved for public release; distribution is unlimited.

Acknowledged Federal Support: **N**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published

Journal: MRS Advances

Publication Identifier Type: DOI

Publication Identifier: 10.1557/adv.2018.405

Volume: Issue:

First Page #: 1

Date Submitted: 7/20/18 12:00AM

Date Published: 4/1/18 12:00AM

Publication Location: Warrendale PA

Article Title: Thermal Evaporated Bismuth Triiodide (BiI₃) Thin Films for Photovoltaic Applications

Authors: Natália F. Coutinho, Rafael B. Merlo, Nelson F. V. Borrero, Francisco C. Marques

Keywords: perovskites photovoltaic physical vapor deposition (PVD) thin film optical properties

Abstract: Bismuth triiodide (BiI₃) is a potential candidate for application in solar cell due to its good optoelectronic properties and because it is free of toxic elements. It can be used as the absorber material in solar cells or converted into the perovskite-like material MA₃Bi₂I₉, suitable also for photovoltaic applications. Bismuth triiodide has been prepared by physical vapour transport (PVT) and by solution process through spin coating. In this work we present optical and structural/topological properties of BiI₃ deposited by thermal evaporation under high vacuum. The films are slightly tensile, polycrystalline, homogeneously distributed and with good adherence on several substrates, with an indirect bandgap of 1.81 eV, index of refraction of 3.3 (630 nm), photoluminescence centered at 1.74 eV and a Raman peak at 118cm⁻¹ associated with the Ag mode.

Distribution Statement: 1-Approved for public release; distribution is unlimited.

Acknowledged Federal Support: **N**

RPPR Final Report as of 17-Sep-2018

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Volume: Issue:

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Date Submitted: 7/20/18 12:00AM

Date Published: 6/1/18 12:00AM

Publication Location: Warrendale PA

Article Title: Dynamics, Design, and Application of a Silicon-on-Insulator Technology Based Neuron

Authors: S. Dutta, T. Chavan, S. Shukla, V. Kumar, A. Shukla, N. Mohapatra, U. Ganguly

Keywords: electrical properties Si

Abstract: Spiking Neural Networks propose to mimic nature's way of recognizing patterns and making decisions in a fuzzy manner. To develop such networks in hardware, a highly manufacturable technology is required. We have proposed a silicon-based leaky integrate and fire (LIF) neuron, on a sufficiently matured 32 nm CMOS silicon-on-insulator (SOI) technology. The floating body effect of the partially depleted (PD) SOI transistor is used to store "holes" generated by impact ionization in the floating body, which performs the "integrate" function. Recombination or equivalent hole loss mimics the "leak" functions. The "hole" storage reduces the source barrier to increase the transistor current. Upon reaching a threshold current level, an external circuit records a "firing" event and resets the SOI MOSFET by draining all the stored holes. In terms of application, the neuron is able to show classification problems with reasonable accuracy. We looked at the effect of scaling experimentally.

Distribution Statement: 1-Approved for public release; distribution is unlimited.

Acknowledged Federal Support: **N**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published

Journal: MRS Advances

Publication Identifier Type: DOI

Publication Identifier: 10.1557/adv.2018.429

Volume: Issue:

First Page #: 1

Date Submitted: 7/20/18 12:00AM

Date Published: 5/1/18 12:00AM

Publication Location: Warrendale PA

Article Title: The Internal Buckling Behavior Induced by Growth Self-restriction in Vertical Multi-walled Carbon Nanotube Arrays

Authors: Quan Zhang, Guo-an Cheng, Rui-ting Zheng

Keywords: structural stress/strain relationship plasma-enhanced CVD (PECVD) (deposition) interface nanostructure

Abstract: The internal buckling is a common phenomenon in the as-grown carbon nanotube arrays. It makes the physical properties of carbon nanotube array in experiment lower than that in theory. In this work, we analyzed the formation and evolution mechanism of the internal buckling based on quasi-static compression model, which is different from collective effect of the van der Waals interactions. The self-restriction effect and the different growth rate of carbon nanotubes verify the possibility of the quasi-static compression model to explain the morphology evolution of vertical carbon nanotube arrays, especially the phenomenon of the quasi-straight and bent carbon nanotubes coexisted in the array. We generalized the Euler beam to wave-like beam and explained the mechanism of high-mode buckling combined with the van der Waals interaction.

Distribution Statement: 1-Approved for public release; distribution is unlimited.

Acknowledged Federal Support: **N**

Technical Report

Grant Number: W911NF-18-1-0154

Amount: \$5,000

Reporting Period: 3 April 2018 to 2 September 2018

Funded symposium: MRS 2018 Spring Meeting in Phoenix, Symposium EN15 - Novel Materials Physics of Perovskite Semiconductors

Objectives:

In the past several years, halide perovskite materials have been shown to exhibit extraordinary performance as photovoltaic materials. It has been revealed that novel material physics is behind the success of these materials. For example, ultra-long carrier lifetime has rarely been observed in other semiconductor materials. Considering that these materials are prepared by low-cost solution-based methods, the finding is even more surprising. Understanding such a highly desired property is not only essential to the further development of these materials for applications, but also enriches our knowledge base generally applicable to other semiconductor materials. Achieving this goal requires synergetic efforts from synthesis of high-quality materials, delicate characterization of their properties, as well as understanding of the physical processes from theory and computation. This symposium was dedicated to understanding perovskite semiconductors from their fundamental physics and materials science aspects.

Presentations

Symposium EN15 received about 110 submissions, of which 94 were accepted. Among the accepted presentations, 22 were invited, 54 were contributed oral presentations, and 18 were posters. The titles of the invited presentations are:

Mercouri Kanatzidis, 3D and 2D Halide Perovskites - Poor Man's High Performance Semiconductors

Jian Shi, Low Dimensional Soft Perovskite Crystals

Wanyi Nie, The Interplay of Structure, Light and Electric Field in 3D and 2D Perovskite Photovoltaic Devices

Nam-Gyu Park, Non-Heating, Large-Area Coating Technology for High Efficiency Perovskite Solar Cells

Henry Snaith, Understanding Instability and Enhancing the Stability of Metal Halide Perovskite Solar Cells

Osman Bakr, Understanding the Origins of Ultra-long Radiative States in Metal Halide Perovskite Crystals

Annamaria Petrozza, Understanding Defect Physics in Metal Halide Perovskite Semiconductors

Hemamala Karunadasa, Capturing the Properties of Lead Halide Perovskites with New Materials

David Mitzi, Structural Diversity and Engineering within Layered Halide Perovskite Semiconductors

Yabing Qi, Perovskite Material and Solar Cell Research by Surface Science and Advanced Characterization

Leeor Kronik, Structural Dynamics in Lead Halide Perovskites from First Principles

Xiaoyang Zhu, Solving the Lead Halide Perovskite Puzzle

Prashant Kamat, Charging Effects in TiO₂ and Its Influence on the Carrier Recombination in CsPbBr₃ Perovskite Films

Oleg Prezhdo, Excited State Dynamics of Photo-excited Charge Carriers in Halide Perovskites - Time Domain Ab Initio Studies

Yanfa Yan, Oxide Double Perovskites for Efficient Photoelectrochemical Water Oxidation

Felix Deschler, Probing the Origin of Strong Radiative Band Edge Emission in Hybrid Perovskites with Ultrafast Spectroscopy

Lijun Zhang, Computational Design of Lead-free Halide Perovskites for Solar Application

Mao-Hua Du, Low-Dimensional Hybrid Organic-Inorganic Metal Halides as Efficient Luminescent Materials

Yoshihiko Kanemitsu, Exciton Dynamics in Lead Halide Perovskite Nanocrystals

Filippo De Angelis, Dielectric Screening and Exciton Binding Energy in Metal Halide Perovskites

Daniel Niesner, Giant Rashba Splitting in Lead Halide Perovskite

Peijun Guo, Ultrafast and First Principles Investigations of Carrier and Phonon Dynamics in Perovskite Halides

Highlights

Some unique physical properties of the hybrid halide perovskites that contribute to the high power conversion efficiency have been revealed theoretically and experimentally over the past several years. Among others, these materials exhibit high defect tolerance so that defect-mediated recombination could be weaker than radiative recombination [*Talk by Annamaria Petrozza*]. Even the radiative recombination could be significantly reduced by screening effect, which forms the so-called large polarons. It was originally perceived that the polarons are formed by the nearly freely rotating dipolar cations. However, the “soft” nature of such materials [*Talk by Leeor Kronik*] actually leads to the understanding that the polarons are most probably a result of the Pb-I framework [*Talk by Xiaoyang Zhu*]. Making high-PCE solar cells is a battle with recombination. With these highly desired properties which reduce recombination, there is reason to be enthusiastic to further push the limit towards higher efficiency, ideally reaching the Shockley-Queisser limit, and eventually industrial application.

Contributions to discipline

Defect tolerant semiconductors have long been searched for various applications, especially for photovoltaics, where low cost is a critical criterion to satisfy if aiming at large-scale applications. The organic-inorganic hybrid halide perovskites have appeared to be the first material that fulfills the criterion. This is a significant contribution to the theory and application of semiconductor materials. The understandings on the halide perovskites may lead to discovery of new semiconductor materials for broader applications.

Formation of polarons typically leads to low carrier mobility, which is usually undesired. Ionic semiconductors are therefore overlooked for mainstream semiconductor applications. However, in halide

materials, the large polarons prevent the recombination of electrons and holes and, therefore, significantly increase the carrier lifetime, which compensates the relatively low mobilities and eventually yields ultra-long carrier diffusion length. These findings open a new venue for the future design of novel semiconductor materials for various applications.

Future direction of this symposium topic

This symposium is the first time when the physics part on perovskite photovoltaics is spun off from the device part in an MRS meeting. The idea was to summarize the unique material physics that we have learned from the hybrid halide perovskites with a hope to transplant such understanding to the development of other semiconductor materials. This symposium topic has been carried on in the forthcoming 2018 MRS Fall Meeting in Boston.

List of supported speakers, symposium chairs and session chairs

Zhu, Xiaoyang (Invited speaker)

Park, Nam-Gyu (Invited speaker)

Zhang, Lijun (Invited speaker)

Mitzi, David (Invited speaker)

Shi, Jian (Invited speaker)

Prezhdo, Oleg (Invited speaker)

Karunadasa, Hemamala (Invited speaker)

Zeng, Hao (Invited speaker)

Guo, Peijun (Invited speaker)

Du, Maohua (Invited speaker)

Deschler, Felix (Invited speaker)

Kronik, Leeor (Invited speaker)

Neisner, Daniel (Invited speaker)

Qi, Yabing (Invited speaker)

Xiao, Zewen (Session chair)

Zhou, Yuanyuan (Session chair)

Petrozza, Annamaria (Invited speaker)

Saparov, Bayrammurad (Symposium chair)

Sun, Yiyang (Symposium chair)

SYMPOSIUM EN15

Novel Materials Physics of Perovskite Semiconductors
April 2 - April 6, 2018

Symposium Organizers

Mingzhen Liu, University of Electronic Science
and Technology
Bayrammurad Saparov, University of Oklahoma
Aron Walsh, Imperial College London
Sun Yi-Yang, Shanghai Institute of Ceramics, Chinese
Academy of Sciences

MRS Invitation to Publish

All authors are invited to submit articles based on their 2018 MRS Spring Meeting presentations to journals in the MRS portfolio. (www.mrs.org/publications-news) Papers submitted and accepted for publication in MRS Advances (www.mrs.org/mrs-advances) will be available as symposium collections. Visit the MRS/Cambridge University Press Publications Booth #100 in the Exhibit Hall to learn more, including MRS Advances print options available at special rates during the meeting week only.

* Invited Paper

SESSION EN15.01: Low-Dimensional Perovskites
Session Chairs: Yi-Yang Sun and Aron Walsh
Monday Afternoon, April 2, 2018
PCC North, 100 Level, Room 122 C

1:30 PM *EN15.01.01
3D and 2D Halide Perovskites—Poor Man's High Performance Semiconductors Mercouri G. Kanatzidis; Northwestern University, United States.

2:00 PM *EN15.01.02
Low-Dimensional Soft Perovskite Crystals Jian Shi; Rensselaer Polytechnic Institute, United States.

2:30 PM EN15.01.03
Structures and Properties of New 2D Lead Halide Perovskites with a Conjugated Diammonium Matthew P. Hautzinger; University of Wisconsin Madison, United States.

2:45 PM EN15.01.04
Identifying the Bandgap of Two-Dimensional Perovskite CsPb₂Br₃ Jiming Bao^{1,2}; ¹University of Houston, United States; ²University of Electronic Science and Technology of China, China.

3:00 PM BREAK

3:30 PM *EN15.01.05
The Interplay of Structure, Light and Electric-Field in 3D and 2D Perovskite Photovoltaic Devices Wanyi Nie; Los Alamos National Laboratory, United States.

4:00 PM EN15.01.06
Electron-Phonon Coupling and Slow Vibrational Relaxation in 2D Organic-Inorganic Hybrid Perovskites Daniel B. Straus; University of Pennsylvania, United States.

4:15 PM EN15.01.07
Improving the Stability of the Hybrid Perovskites—A New Structural Motif Alex M. Ganose^{1,2}; ¹University College London, United Kingdom; ²Diamond Light Source, United Kingdom.

4:30 PM EN15.01.08
Novel Hybrid Organic-Inorganic Electron Extraction Layers for Polymer Solar Cells with Improved Processing Robustness Donia Fredj^{3,4}; ³Faculté des sciences de Sfax, France; ⁴Faculté des sciences de Sfax, Tunisia.

4:45 PM EN15.01.09
Band Tail States in FAPbI₃—Characterization and Simulation Adam D. Wright; Department of Physics, University of Oxford, United Kingdom.

SESSION EN15.02: Device Physics
Session Chair: Mingzhen Liu
Tuesday Morning, April 3, 2018
PCC North, 100 Level, Room 122 C

10:30 AM *EN15.02.01
Non-Heating, Large-Area Coating Technology for High Efficiency Perovskite Solar Cells Nam-Gyu Park; Sungkyunkwan University, Korea (the Republic of).

11:00 AM *EN15.02.02
Cubic Perovskite Semiconductors with Enhanced Photovoltaic Properties Peng Qin; Shanghai Institute of Ceramics, Chinese Academy of Sciences, China.

11:30 AM *EN15.02.03
Understanding Instability and Enhancing the Stability of Metal Halide Perovskite Solar Cells Henry Snaith; University of Oxford, United Kingdom.

SESSION EN15.03: Defect Properties
Session Chairs: Bayrammurad Saparov and Zewen Xiao
Tuesday Afternoon, April 3, 2018
PCC North, 100 Level, Room 122 C

1:30 PM EN15.03.01
Defect Properties of Halide Double Perovskite Semiconductors Zewen Xiao; Tokyo Institute of Technology, Japan.

1:45 PM EN15.03.02
The Unusual Character of Point Defects in Organic-Inorganic Perovskite Solar Cells Olivia D. Hentz; Massachusetts Institute of Technology, United States.

2:00 PM *EN15.03.03
Understanding the Origins of Ultralong Radiative States in Metal Halide Perovskite Crystals Osman M. Bakr; KAUST, Saudi Arabia.

2:30 PM BREAK

3:30 PM EN15.03.04
Effects of A-Site Symmetry-Breaking and Dynamically Correlated Disorder on Phase Transition and Thermal Properties of Hybrid Organic-Inorganic Perovskites Taishan Zhu; Univ of Illinois-Urbana Champ, United States.

3:45 PM EN15.03.05
Role of Lead Vacancies for Optoelectronic Properties of Lead-Halide Perovskites Dmitri Kilin^{1,2}; ¹University of South Dakota, United States; ²North Dakota State University, United States.

4:00 PM *EN15.03.06
Understanding Defect Physics in Metal-Halide Perovskite Semiconductors Annamaria Petrozza; Istituto Italiano di Tecnologia, Italy.

4:30 PM EN15.03.07
Defect Physics of Lead-Based Mixed Halide Hybrid Perovskites from First Principles Computations Arun Kumar Mannodi Kanakkithodi; Argonne National Laboratory, United States.

4:45 PM EN15.03.08
Charge-Carrier Traps in Hybrid Perovskites and the Consequences for Solar Cells Moritz H. Futscher; AMOLF, Netherlands.

SESSION EN15.04: Novel Perovskites
Session Chairs: Bayrammurad Saparov and Yi-Yang Sun
Wednesday Morning, April 4, 2018
PCC North, 100 Level, Room 122 C

8:00 AM EN15.04.01
Design Lead-Free Organic-Inorganic Double Perovskites for Optoelectronics—A High-Throughput Approach Kesong Yang; University of California, San Diego, United States.

8:15 AM EN15.04.02
Materials Discovery—From Bi-Based to Rare-Earth Hybrid Double Perovskites Zeyu Deng; University of Cambridge, United Kingdom.

8:30 AM *EN15.04.03
Capturing the Properties of Lead-Halide Perovskites with New Materials Hemamala Karunadasa; Stanford University, United States.

9:00 AM *EN15.04.04

Chalcogenide Perovskite—An Emerging Ionic Semiconductor for PV Applications Hao Zeng; SUNY-Buffalo, United States.

9:30 AM BREAK

10:00 AM EN15.04.05

A'A'TeBiO₆—A New Family of Inorganic Double Perovskite Oxides Containing Bismuth for Photovoltaic Applications Arashdeep S. Thind; Washington University in St. Louis, United States.

10:15 AM EN15.04.06

All-Inorganic Titanium-Based Halide Perovskite Solar Cells Min Chen; Brown University, United States.

10:30 AM EN15.04.07

Verification the Surface State of Cs₂SnI₆ as a Main Charge Transfer Pathway HyeonOh Shin; Ulsan National Institute of Science and Technology, Korea (the Republic of).

10:45 AM EN15.04.08

Fast Search for Novel Materials Enabled by Transfer Learning Matthias Poloczek; University of Arizona, United States.

11:00 AM *EN15.04.09

Structural Diversity and Engineering within Layered Halide Perovskite Semiconductors David B. Mitzi; Duke University, United States.

11:30 AM EN15.04.10

Aziridinium Lead Iodide—A New, Stable, Low Bandgap Hybrid Halide Perovskite for Photovoltaics Chao Zheng; McMaster University, Canada.

11:45 AM EN15.04.11

Determination of Adsorption-Controlled Growth Windows of Chalcogenide Perovskites Rafael Jaramillo; Massachusetts Institute of Technology, United States.

SESSION EN15.05: Advanced Characterization

Session Chair: Lijun Zhang

Wednesday Afternoon, April 4, 2018

PCC North, 100 Level, Room 122 C

1:30 PM EN15.05.01

Time-Resolved X-Ray Absorption Near Edge Structure (TR-XANES) Spectroscopy of Lead-Free Perovskite Nanocrystals Cunming Liu; Argonne National Laboratory, United States.

1:45 PM EN15.05.02

Photocurrent Spectroscopy of Thermally Evaporated Perovskite Solar Cells Jay Patel; University of Oxford, United Kingdom.

2:00 PM *EN15.05.03

Perovskite Material and Solar Cell Research by Surface Science and Advanced Characterization Yabing Qi; Okinawa Institute of Science and Technology, Japan.

2:30 PM BREAK

3:30 PM EN15.05.04

Probing Electron-Phonon Interactions in Single Crystalline van der Waals Ruddlesden-Popper Perovskite (C₄H₉NH₃)₂PbI₄ Prepared by Vapor Deposition Zhizhong Chen; Rensselaer Polytechnic Institute, United States.

3:45 PM EN15.05.05

Spatial-Temporal Spectroscopy and Electronic Structure of Methyl Ammonium Perovskites Rana Biswas^{1,2}; ¹Iowa State University, United States; ²Ames Laboratory, United States.

4:00 PM *EN15.05.06

Structural Dynamics in Lead-Halide Perovskites from First-Principles Leor Kronik; Weizmann Institute of Science, Israel.

4:30 PM EN15.05.07

Slow Thermal Equilibration in Hybrid Organic-Inorganic Perovskites Revealed by Transient Infrared Absorption Spectroscopy Peijun Guo; Argonne National Laboratory, United States.

4:45 PM EN15.05.08

Development of Low-Energy Ultraviolet and Inverse Photoelectron Spectroscopies and Their Application To Determining Energy Levels in Organometal Halide Perovskites Kenneth R. Graham; University of Kentucky, United States.

SESSION EN15.06: Poster Session I: Material Physics of Perovskites

Session Chair: Yi-Yang Sun

Wednesday Afternoon, April 4, 2018

5:00 PM - 7:00 PM

PCC North, 300 Level, Exhibit Hall C-E

EN15.06.01

Systematic Modelling of Electronic Properties of ABX₃ Perovskites Dani Metin; The University of Auckland, New Zealand.

EN15.06.02

Overcoming Recombination Limited Photocurrent Generation in CsPbX₃ Nanocrystal Based Arrays Wasim J. Mir^{1,2}; ¹Department of Chemistry, Indian Institute of Science Education and Research (IISER), India; ²Sorbonne Universités, UPMC Univ. Paris 06, CNRS-UMR 7588, Institut des NanoSciences de Paris, France.

EN15.06.03

Photoreponse of All-Inorganic Perovskite Semiconductor—Growth and Characterization of CsPbBr₃ and Cs₄PbBr₆ Single Crystal Ji-Hyun Cha; Sungkyunkwan University, Korea (the Republic of).

EN15.06.04

Understanding the Stability of Mixed A-Cation Lead Iodide Perovskites Bethan Charles; University of Bath, United Kingdom.

EN15.06.05

Visualization and Kinetic Studies of Ion Diffusion in Cesium Lead Bromide Perovskite Nanowires Dongxu Pan; University of Wisconsin, Madison, United States.

EN15.06.06

Ultraviolet and Inverse Photoelectron Spectroscopies for Probing the Electronic Structure of Tin Halide Perovskites Alex Boehm; University of Kentucky, United States.

EN15.06.07

Probing the Occupied and Unoccupied Density of States of Hybrid Perovskites Selina Olthof; University of Cologne, Germany.

EN15.06.08

Enhanced Grain Size and Crystallinity in CH₃NH₃PbI₃ Perovskite Films by Metal Additives to the Single-Step Solution Fabrication Process Zahrah S. Almutawah; University of Toledo, United States.

EN15.06.09

Crystal Lattice Dynamics of the Substituted Solid Solutions in the Bi(Gd)-Fe-O and Bi(Nd)-Fe-O Systems B. Korzun; The City University of New York, United States.

SESSION EN15.07: Carrier Dynamics

Session Chairs: Mao-hua Du and Jian Shi

Thursday Morning, April 5, 2018

PCC North, 100 Level, Room 122 C

8:00 AM EN15.07.01

Efficient Photon Recycling and Radiation Trapping in Cesium Lead Halide Perovskite Microwire Waveguides Anton Malko; The University of Texas at Dallas, United States.

8:15 AM EN15.07.02

Understanding and Exploring the Hidden Photo Physics and Carrier Dynamics in Epitaxial Halide Perovskite Nanostructure and Thin Film Yiping Wang; Rensselaer Polytechnic Institute, United States.

8:30 AM *EN15.07.03

Solving the Lead Halide Perovskite Puzzle Xiaoyang Zhu; Columbia University, United States.

9:00 AM *EN15.07.04

Charging Effects in TiO₂ and Its Influence on the Carrier Recombination in CsPbBr₃ Perovskite Films Prashant Kamat; University of Notre Dame, United States.

9:30 AM EN15.07.05

The Final Limit—Investigating the Mechanism Between Absorption and Bimolecular Recombination in Hybrid Metal Halide Perovskites Christopher L. Davies; University of Oxford, United Kingdom.

9:45 AM BREAK

10:15 AM EN15.07.06

Carrier Dynamics in Methylammonium Lead Iodide Studied Using Low Optical Power Density, Steady-State Microwave Conductivity
John G. Labram; Oregon State University, United States.

10:30 AM *EN15.07.07

Excited State Dynamics of Photoexcited Charge Carriers in Halide Perovskites—Time-Domain *Ab Initio* Studies Oleg Prezhdo; University of Southern California, United States.

11:00 AM EN15.07.08

Ultrafast Excited-State Dynamics in Shape- and Composition-Controlled CsPbX₃ Nanocrystals Naiya Soetan; Vanderbilt University, United States.

11:15 AM EN15.07.09

The Influence of Cation Dipole Moment on the Indirect Bandgap in Lead Halide Perovskites Benjamin Daiber; AMOLF, Netherlands.

11:30 AM EN15.07.10

Exploring the Way to Approach the Efficiency Limit of Perovskite Solar Cells by Drift-Diffusion Model Wallace C. Choy; University of Hong Kong, China.

11:45 AM EN15.07.11

The Novel Dopant for Hole-Transporting Material Opens a New Processing Route to Efficiently Reduce Hysteresis and Improve Stability of Planar Perovskite Solar Cells Junsheng Luo; University of Electronic Science and Technology of China, China.

SESSION EN15.08: Novel Applications
Session Chairs: Mingzhen Liu and Bayrammurad Saparov
Thursday Afternoon, April 5, 2018
PCC North, 100 Level, Room 122 C

1:30 PM EN15.08.01

Environmental Studies of Perovskite Solar Cells for Space Applications
Pilar Espinet Gonzalez; California Institute of Technology, United States.

1:45 PM *EN15.08.02

Oxide Double Perovskites for Efficient Photoelectrochemical Water Oxidation Yanfa Yan; University of Toledo, United States.

2:15 PM EN15.08.03

PEDOT/NiO Composite Hole Transportation Layer for Perovskite Solar Cells Joseph Asare^{1,2,3}; ¹Baze University, Nigeria; ²Arizona State University, United States; ³African University of Science and Technology (AUST), Nigeria.

2:30 PM BREAK

3:30 PM EN15.08.04

Multiphoton Absorption Order of CsPbBr₃ as Determined by Wavelength-Dependent Nonlinear Optical Spectroscopy Joon Jang; Sogang University, Korea (the Republic of).

3:45 PM EN15.08.05

Origin of Performance Enhancement in Single-Walled Carbon Nanotube Loaded Mesoporous TiO₂ Perovskite Solar Cells Thomas J. MacDonald; University College London, United Kingdom.

4:00 PM *EN15.08.06

Probing the Origin of Strong Radiative Band Edge Emission in Hybrid Perovskites with Ultrafast Spectroscopy Felix Deschler; Univ of Cambridge, United Kingdom.

4:30 PM EN15.08.07

A Novel Non-Halide Lead Source for High Efficiency Perovskite Solar Cells Faming Li; University of Electronic Science and Technology of China, China.

4:45 PM EN15.08.08

Ferroelectric Domains in Methylammonium Lead Iodide Thin-Film Solar Cells Alexander Colmann; Karlsruhe Institute of Technology, Germany.

SESSION EN15.09: Poster Session II
Thursday Afternoon, April 5, 2018
5:00 PM - 7:00 PM
PCC North, 300 Level, Exhibit Hall C-E

EN15.09.01

Surface-Guided CsPbBr₃ Perovskite Nanowires with Size-Dependent Photoluminescence Well Beyond the Quantum Confinement Regime Eitan Oksenberg; Weizmann Institute of Science, Israel.

EN15.09.02

Ambipolar Alpha Particle Detection in the A₃M₂I₉ Defect Perovskites Kyle M. McCall^{1,2}; ¹Northwestern University, United States; ²Northwestern University, United States.

EN15.09.03

Lead-Free, Stable and Sensitive X-Ray Detectors Based on Cs₂AgBiBr₆ Single Crystal and Wafer Jiang Tang; Wuhan National Laboratory for Optoelectronics, China.

EN15.09.05

Vis-Near Infrared Photodetectors Based on Methyl Ammonium Lead Iodide Thin Films by Pulsed Laser Deposition Nagabhushan Patel; Indian Institute of Science, India.

EN15.09.06

Lead-Free Perovskites Thin Films Obtained by Pulsed Laser Deposition and Their Functional Properties Andreea Carmen Andrei; NILPRP, Romania.

EN15.09.07

Halide Migration and Phase Stability in Mixed-Halide Organic-Inorganic Perovskite Heterostructures Rhiannon (Rhys) M. Kennard; University of California, Santa Barbara, United States.

EN15.09.08

Prediction of Crystal Structure of Hybrid Organic-Inorganic Perovskite by First-Principles Evolutionary Technique Omotayo A. Salawu; Korea Institute of Energy Research, Korea (the Republic of).

EN15.09.09

Seamless Stitching Between Single All-Inorganic Perovskite Nanocrystals Leyre Gomez; Institute of Physics, Netherlands.

EN15.09.10

Thermal Evaporated Bismuth Triiodide (BiI₃) Thin Films for Photovoltaic Applications Natalia d. Coutinho; UNICAMP, Brazil.

EN15.09.11

Bandgap Tuning of Organo-Metal Halide Perovskite in Ternary Phase Diagram Si Hong Lee; Kyungpook National University, Korea (the Republic of).

SESSION EN15.10: Structure and Growth
Session Chairs: Xujie Lu and Yuanyuan Zhou
Friday Morning, April 6, 2018
PCC North, 100 Level, Room 122 C

8:00 AM EN15.10.01

Microstructural/Compositional Tailoring of Cesium Tin Iodide Perovskites for Solar Cells with Improved Efficiency and Stability Yuanyuan Zhou; Brown University, United States.

8:15 AM *EN15.10.02

Computational Design of Lead-free Halide Perovskites for Solar Application Lijun Zhang; College of Materials Science and Engineering, Jilin University, China.

8:45 AM *EN15.10.03

Pressure-Induced Dramatic Changes in Structures and Properties of Halide Perovskites Xujie Lu; Center for High Pressure Science and Technology Advanced Research, China.

9:15 AM EN15.10.04

Methylammonium Iodide Effect on the Supersaturation Concentration and Interfacial Energy of the Crystallization of Methylammonium Lead Triiodide Single Crystals Bichen Li; National University of Singapore, Singapore.

9:30 AM BREAK

10:00 AM EN15.10.05

Effect of Excessive Lead on the Stability and Performance of Lead Halide Perovskite Solar Cells Against Photo-Induced Degradation Aditya S. Yerramilli; Arizona State University, United States.

10:15 AM EN15.10.06

Impact of Organic Cation Dynamics on Solar Cell Performance of Metal Halide Perovskites Joshua Choi; University of Virginia, United States.

10:30 AM EN15.10.07

Elucidating the Photoinstability and Degradation Kinetics of Organic-Inorganic Halide Perovskites Zhaoning Song; University of Toledo, United States.

10:45 AM *EN15.10.08
Low-Dimensional Hybrid Organic-Inorganic Metal Halides as Efficient Luminescent Materials Mao-hua Du; Oak Ridge National Laboratory, United States.

11:15 AM EN15.10.09
Toward Capillary-Fed Solution Growth of Thin, Monocrystalline Perovskite Films Genevieve Hall; Arizona State University, United States.

11:30 AM EN15.10.10
Investigation of Post Deposition Annealing Temperature Effect on the Performance of Dehydrated Lead Acetate Precursor in an Inverted Planar $\text{CH}_3\text{NH}_3\text{PbI}_3$ Perovskite Solar Cells Aditya S. Yerramilli; Arizona State University, United States.

11:45 AM EN15.10.11
The Presence and Impact of Ferroelectricity in Methylammonium Lead Iodide Lauren Garten; NREL, United States.

SESSION EN15.11: Exciton and Many-Body Effect
Session Chair: Yi-Yang Sun
Friday Afternoon, April 6, 2018
PCC North, 100 Level, Room 122 C

1:30 PM *EN15.11.01
Exciton Dynamics in Lead Halide Perovskite Nanocrystals Yoshihiko Kanemitsu; Kyoto University, Japan.

2:00 PM *EN15.11.02
Dielectric Screening and Exciton Binding Energy in Metal-Halide Perovskites Filippo De Angelis^{1,2}; ¹CNR-ISTM, Italy; ²Istituto Italiano di Tecnologia, Italy.

2:30 PM BREAK

3:00 PM EN15.11.03
Band Tailing and Deep Defect States in $\text{CH}_3\text{NH}_3\text{Pb}(\text{I}_{1-x}\text{Br}_x)_3$ Perovskites Carolin M. Sutter-Fella; Lawrence Berkeley National Laboratory, United States.

3:15 PM EN15.11.04
Dephasing and Quantum Beating of Excitons in Methylammonium Lead Iodide Perovskite Nanoplatelets Bernhard J. Bohn; Ludwig-Maximilians-Universität München, Germany.

3:30 PM *EN15.11.05
Giant Rashba Splitting in Lead Halide Perovskite Daniel Niesner; Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Germany.

4:00 PM EN15.11.06
Origin of Abnormal Bandgap Shift and Second Emission Peak in Organic-Inorganic Lead Halide Perovskites M. Ibrahim Dar; Ecole Polytechnique Federale de Lausanne, Switzerland.

4:15 PM *EN15.11.07
First Principles Modeling of Phonon Transport and Equilibration in Perovskite Halides Maria K. Chan; Argonne National Laboratory, United States.

4:45 PM EN15.11.08
Dresselhaus-Rashba Semiconductors in Photovoltaics Combine Benefits of Direct and Indirect Semiconductors Oleg Rubel; McMaster University, Canada.

SYMPOSIUM EN16

Combining Materials, Technologies and Societal Awareness
to Harvest Natural and Human-Made Energy Sources
April 3 - April 5, 2018

Symposium Organizers

Tito Busani, University of New Mexico
Sergej Filonovich, Total Gas
Olga Lavrova, Sandia National Laboratories
Robert Opila, University of Delaware

MRS Invitation to Publish

All authors are invited to submit articles based on their 2018 MRS Spring Meeting presentations to journals in the MRS portfolio. (www.mrs.org/publications-news) Papers submitted and accepted for publication in MRS Advances (www.mrs.org/mrs-advances) will be available as symposium collections. Visit the MRS/Cambridge University Press Publications Booth #100 in the Exhibit Hall to learn more, including MRS Advances print options available at special rates during the meeting week only.

* Invited Paper

SESSION EN16.01: Role of Solar Energy for Renewable Systems I
Session Chairs: Tito Busani and Matthew Doty
Tuesday Morning, April 3, 2018
PCC North, 100 Level, Room 128 A

10:30 AM *EN16.01.01
Scalable and Sustainable Tandem Solar Devices—Low-Cost Tandem Photovoltaics and Tandem Photoelectrodes for Solar Fuel Generation Harry A. Atwater; California Institute of Technology, United States.

11:00 AM *EN16.01.02
Bridging Scientific Research and Industry—Research Progress on Industrial Crystalline Silicon Solar Cells at SJTU Wenzhong Shen; Shanghai Jiao Tong University, China.

11:30 AM EN16.01.03
Aluminum Zinc Oxide (AZO) Optimization Process for Use in Optically Transparent Antennas Maria E. Zamudio; The University of New Mexico, United States.

11:45 AM EN16.01.04
Polymer-Dopant Synergies for Thermoelectric Performance in Sustainable Materials Howard E. Katz; Johns Hopkins University, United States.

SESSION EN16.02: Role of Solar Energy for Renewable Systems II
Session Chairs: Robert Opila and Elizabeth Zamudio
Tuesday Afternoon, April 3, 2018
PCC North, 100 Level, Room 128 A

1:30 PM *EN16.02.01
High Efficiency Photovoltaics as the Basis for a Modern Energy System Christiana Honsberg; Arizona State University, United States.

2:00 PM *EN16.02.02
A New Type of Heat Engine—Using LED's as Refrigerators Eli Yablonovitch; University of California, Berkeley, United States.

2:30 PM BREAK

3:30 PM *EN16.02.03
Addressing the Challenges of Harvesting and Locally Using Solar Energy Alison Lennox; UNSW Sydney, Australia.

4:00 PM *EN16.02.04
Photon Recycling—Upconversion of Low-Energy Photons in Semiconductor Nanostructures Matthew Doty; University of Delaware, United States.

4:30 PM *EN16.02.05
Energy Loss Due to Soiling of Photovoltaic Systems Bruce King; Sandia National Labs, United States.

EP-06: Materials, Devices and Systems for Machine Learning and Neuromorphic Computing

With a paradigm shift in the nature of computational workloads for most applications today, there are significant efforts in devising new information processing engines inspired by the brain that tap into the unique nanoscale and quantum nature of materials. The goal of this symposium was to provide an overview of current active topics of research in materials science targeted at developing new materials for analytics and neuromorphic computing. The symposium featured invited talks from researchers that provided a high-level view of machine learning trends, and requirements from systems development perspective, as well as cutting-edge developments in new materials systems such as memristors, chalcogenides, polymers and organic materials.

Keynote speakers: The symposium had the following keynote talks, covering basic materials and device optimization for deep learning applications, system optimization perspective as well as algorithmic aspects for learning systems beyond deep learning:

1. Dr. Geoff Burr, IBM Almaden, *Neuromorphic Computation for Hardware Acceleration of Deep Neural Networks - Challenges and Perspectives*
2. Dr. Dileep George, CEO of Vicarious Inc, *What is Beyond Deep and Narrow for AI?*
3. Prof. Subhasish Mitra, Stanford University, *Transforming Nanodevices into NanoSystems - The N3XT 1,000X*

Invited speakers: The symposium also featured invited talks from the following speakers, covering a wide spectrum of topics ranging from basic materials optimization to system level implementation:

1. Prof. Subu Iyer, UCLA, *Technologies for Massively Scaled-Out Neuromorphic Systems (MaSoNs)*
2. Prof. Hyunsang Hwang, Pohang University of Science and Technology, *ReRAM Based Synapse Devices and IMT Oscillator Neuron for Neuromorphic System*
3. Dr. Xavier Obradors, Institute of Materials Science of Barcelona, *Resistive Switching Mechanism in Metallic Perovskite Thin Film Oxides Displaying Metal Insulator Transitions*
4. Dr. Fabien Alibart, French National Centre for Scientific Research, *Neuromorphic Computing—Toward Dynamical Data Processing*
5. Prof. Udayan Ganguly, IIT Bombay, *Dynamics, Design and Application of a Silicon on Insulator Technology Based Neuron*
6. Dr. Alice Mizrahi, NIST, *Neural-Like Computing with Populations of Superparamagnetic Basis Functions*
7. Dr. Suhas Kumar, HP Labs, *Memristor Based Analog Computations - Devices, Systems and Experimental Demonstrations*
8. Dr. Alex Serb, University of Southampton, *Processing Big Data with Metal Oxide Memristors*
9. Dr. Angel Yanguas Gil, Argonne National Laboratory, *Neuromorphic Architectures for Smart Sensing Applications - Lessons from the Insect Brain*
10. Robert Legenstein, TU Graz, *Rewiring in Deep Neural Networks with Noisy Parameter Updates*
11. Jennifer Rupp, MIT, *Oxide Architectures and Defect Design for Next Materials in Neuromorphic Computing*
12. Blanka Magyari Kope, Stanford, *Non-Volatile Memory Device Optimization Trends from Ab Initio Simulations*

13. Sabina Spiga, Institute for microelectronics and microsystems, Italy, *Analog HfO₂-Based Memristive Devices for Spiking Neural Networks*
14. Han Wang, USC, *Emerging 2D Material Devices for Neuromorphic Computing*

Regular talks: The symposium also featured regular talks from the following speakers, covering various fundamental advances in nanoscale device phenomena for neuro-inspired and machine learning-inspired Computing as well as the theory and modeling of material systems for these applications:

1. Elliot Fuller, *Floating Gate Memory Based on Ion Insertion Electrodes for Low Voltage Analog Computing*
2. Sanjoy Nandi, *Evolution of Switching Behaviour in Ag:HfO₂ Based Conductive Bridge RAM Devices*
3. Yuhan Shi, *Modeling Resistive Synaptic Devices for Implementation of Unsupervised Learning with Spiking Neural Networks*
4. Scott Tan, *Epitaxial Silicon-Germanium Artificial Synapses for Neuromorphic Computing Systems*
5. Zheng Wang, *Ferroelectric Coupled Oscillator Network for Neuromorphic Computing*
6. Rohit John, *Flexible Ionic/Electronic Hybrid Oxide Synaptic TFTs with Programmable Dynamic Plasticity for Brain-Inspired Neuromorphic Computing*
7. Yan Fang, *Increasing Information Storage Capacity in Computing Devices Formed from Self-Oscillating Gels*
8. Jun Tao, *Scalable Neuromorphic Computing Platform Based on Indium Phosphide Synaptic Device on Silicon*
9. Sayani Majumdar, *Organic Ferroelectric Memristors for Neuromorphic Computing*
10. Paddy K. L. Chan, *Neuromorphic Computing by Organic Transistor Circuits*
11. Mohammad Sharbati, *Low Power, Electrochemically Tunable Graphene Synapses for Neuromorphic Computing*
12. Akira Sakai, *Demonstrative Operation of Four-Terminal Memristive Devices by Controlling Oxygen Vacancy Distribution in TiO_{2-x} Single Crystals*
13. Amitesh Kumar, *Synaptic Learning and Memory Functions in Amorphous Yttria-Based Memristive Systems*
14. Rohit John, *Hybrid Synaptic Elements for OptoNeuromorphic Computing*
15. Sung Pyo Park, *Investigation of Resistive Switching Behavior for Glucose Based Biomaterials*
16. Brajendra Sengar, *Synaptic Functions Revealed in Dual Ion Beam Sputtered Zinc Oxide Based Memristive Devices for Neuromorphic Computing*

Posters: A poster session was also part of the symposium, with the following 9 posters:

1. Paul Yang, *Single and Double Gate Synaptic Transistors with a Reversible and Analog Drain Current Modulation Using a Pt/HfOx/nIGZO Memcapacitor*
2. Jennifer Gerasimov, *Long and Short Term Potentiation and Depression in an Organic Electronic Synapse*
3. Sung Il Kim, *Artificial Synapse Based on Polymer Blended Perovskite*
4. Steven McGarry, *Drift-Diffusion Simulation of Coupled Ionic-Electronic Devices*

5. Changsheng Wu, *Keystroke Dynamics Enabled Authentication and Identification Using Triboelectric Nanogenerator Array*
6. Geon Won Beom, *Analog Memcapacitance Characteristics in Al/SiO₂/TaOx/nIGZO Capacitor Structure for Synaptic Transistor*
7. Sanjoy Nandi, *Scaling Behaviour and Anatomy of Filamentary Threshold Switching in NbOx*
8. Dashan Shang, *A Synaptic Transistor Based on TwoDimensional Molybdenum Oxide*
9. Armantas Melianas, *Polymer-Based NonVolatile Analog Synapses for Low-Power Neuromorphic Computing*

Contributions to discipline: The keynote talks provided a high level view of the requirements and specifications from nanoscale materials for accelerating future machine learning and neuromorphic algorithms, and for their adaptation at the system level. Talks from senior researchers from IBM and HP clearly laid out some of the requirements as well as approaches to be avoided to engineer nanoscale materials for these applications.

Recent breakthroughs such as the demonstration of using superparamagnetic basis functions for neural like computations (Nature Communications, 2018) and epitaxial SiGe synapses with engineered dislocations (Nature Materials, 2018) were also presented and discussed in detail by the authors at this meeting.

Future direction: The symposium was very well received, and most sessions drew between 30-50 participants. In this highly dynamic and emerging field, it is also crucial that researchers working at materials and device engineering aspects have opportunities to interact and learn from experts in system design and software, so that their research efforts are steered in the right direction. Given that the research into the development of materials and devices for Machine Learning and Neuromorphic Computing is expected to grow in the coming years, the organizers feel that similar symposia should be held in the coming years at MRS meetings as well as other premier conferences.

Award recipients: The following speakers were selected for receiving a financial support of \$600 from the ARO award, based on the evaluation of their CV and a brief statement of interest:

1. Alice Mizrahi, Postdoctoral researcher at the National Institute of Standards and Technology
2. Scott Tan, PhD student at MIT
3. Sayani Majumdar, Academy Research Fellow, Department of Applied Physics, Aalto University school of Science
4. Rohit John, PhD Student at Nanyang Technological University (NTU), Singapore
5. Paddy Chan, Associate Professor in the Department of Mechanical Engineering, The University of Hong Kong
6. Sanjoy Nandi, Postdoctoral Fellow, Research School of Physics and Engineering, Australian National University.
7. Sung Pyo Park, Ph.D candidate in the School of Electrical and Electronic Engineering, Yonsei University
8. Alexander Serb, Post-doctoral research fellow University of Southampton

The symposium organizers: The symposium was organized by Dr. Bipin Rajendran (NJIT), Dr. Duygu Kuzum (UCSD), Dr. Manan Suri (IIT Delhi) and Dr. Abu Sebastian (IBM Research - Zurich).

11:15 AM EP05.09.04

Highly Thickness Tolerant Organometal Halide Perovskite-Polymer Composite Thin Films for Efficient Light-Emitting Diodes Xin Shan^{1,2}; ¹Florida State University, United States; ²Florida State University, United States.

11:30 AM EP05.09.05

Efficient Blue Perovskite Light Emitting Diodes Dan Congreve; Rowland Institute at Harvard, United States.

11:45 AM EP05.09.06

Stable and Bright Perovskite Light-Emitting Diodes with High Energy Conversion Efficiency Yanfeng Miao; Nanjing Tech University, China.

SESSION EP05.10: New Types of Nanoscale Emitters—Perovskites and Non-Perovskites

Session Chair: Jiangeng Xue
Friday Afternoon, April 6, 2018
PCC North, 200 Level, Room 223

1:30 PM EP05.10.01

Characterization of Yb Doped Cesium Lead Halide Perovskite Nanocrystals Arnon Lesage; University of Amsterdam, Netherlands.

1:45 PM EP05.10.02

Highly Luminescent Cubic CH₃NH₃PbI₃ Nanocrystals for Efficient Light Emitting Devices Yasser H. Hassan; University of Oxford, United Kingdom.

2:00 PM EP05.10.03

Temperature-Dependent Photoluminescence of CH₃NH₃PbBr₃ Perovskite and Analysis on Its Photo-Physical Properties Heechul Woo; Gwangju Institute of Science and Technology (GIST), Korea (the Republic of).

2:15 PM EP05.10.04

Transport and GHz Phototransport Reaching Recombination Limited Dynamics in CsPbX₃ Nanocrystal Arrays Clement Livache^{1,2}; ¹ESPCI, France; ²Université Pierre et Marie Curie, France.

2:30 PM EP05.10.05

Single Crystal Growth and Characterization of R-M-X Compounds (R = C₆H₅C₄H₄NH₃, C₆(CH₃)₅CH₂N(CH₃)₃; M = Zn, Cd, Hg; X = Cl, Br, I) for Material Applications Rachel Roccanova; University of Oklahoma, United States.

2:45 PM EP05.10.06

Donor and Acceptor Codoping in Silicon Quantum Dots for Efficient and Tunable Near IR Emission Hiroshi Sugimoto; Kobe University, Japan.

3:00 PM BREAK

3:30 PM EP05.10.07

High-Efficiency Optical Gain in Type-II Semiconductor Nanocrystals of Alloyed Colloidal Quantum Wells Burak Guzel Turk^{1,2}; ¹Stanford University, United States; ²Bilkent University, Turkey.

3:45 PM EP05.10.08

First-Principles Engineering of Charged Defects for Two-Dimensional Quantum Technologies Yuan Ping; University of California Santa Cruz, United States.

4:00 PM EP05.10.09

An Add-On Organic Green-to-Blue Photon-Upconversion Layer for Organic Light Emitting Diodes Lorenz Graf von Reventlow; Karlsruhe Institute of Technology, Germany.

4:15 PM EP05.10.10

InP/InGaAs Multi-Quantum Well Nanowires Grown by MOCVD for Light Emitting Device Applications Inseok Yang; The Australian National University, Australia.

4:30 PM EP05.10.11

Polar-Electrode-Bridged Electroluminescent Devices Based on a Novel Isoplanar Structure Xiuru Xu; Peking University Shenzhen Graduate School, China.

4:45 PM EP05.10.12

Development of Flexible Mechanoluminescent Polymeric Based Systems Carlos A. Hernandez; University of Texas Rio Grande Valley, United States.

SYMPOSIUM EP06

Materials, Devices and Systems for Machine Learning and Neuromorphic Computing
April 3 - April 5, 2018

Symposium Organizers

Duygu Kuzum, University of California San Diego
Bipin Rajendran, New Jersey Institute of Technology
Abu Sebastian, IBM, Zurich
Manan Suri, Indian Institute of Technology Delhi

MRS Invitation to Publish

All authors are invited to submit articles based on their 2018 MRS Spring Meeting presentations to journals in the MRS portfolio. (www.mrs.org/publications-news) Papers submitted and accepted for publication in MRS Advances (www.mrs.org/mrs-advances) will be available as symposium collections. Visit the MRS/Cambridge University Press Publications Booth #100 in the Exhibit Hall to learn more, including MRS Advances print options available at special rates during the meeting week only.

* Invited Paper

SESSION EP06.01: Neuromorphic Devices I
Session Chairs: Fabien Alibart and Duygu Kuzum
Tuesday Morning, April 3, 2018
PCC North, 200 Level, Room 221 C

10:30 AM *EP06.01.01

Technologies for Massively Scaled-Out Neuromorphic Systems (MaSoNs) Subramanian Iyer; University of California, Los Angeles, United States.

11:00 AM EP06.01.02

Floating Gate Memory-Based on Ion Insertion Electrodes for Low-Voltage Analog Computing Elliot J. Fuller; Sandia National Laboratories, United States.

11:15 AM EP06.01.03

Observation of Conductance Plateaus in a Molecular Film via Nanometer Control of Phase Boundary Sreetosh Goswami; National University of Singapore, Singapore.

11:30 AM *EP06.01.04

ReRAM-Based Synapse Devices and IMT Oscillator Neuron for Neuromorphic System Hyunsang Hwang; Pohang University of S&T, Korea (the Republic of).

SESSION EP06.02: Resistive Switching Devices
Session Chairs: Udayan Ganguly and Hyunsang Hwang
Tuesday Afternoon, April 3, 2018
PCC North, 200 Level, Room 221 C

1:30 PM *EP06.02.01

Resistive Switching Mechanism in Metallic Perovskite Thin-Film Oxides Displaying Metal-Insulator Transitions Xavier Obradors; ICAMAB - CSIC, Spain.

2:00 PM EP06.02.02

Evolution of Switching Behaviour in Ag:HfO₂ Based Conductive-Bridge RAM Devices Sanjoy K. Nandi; Australian National University, Australia.

2:15 PM EP06.02.03

Modeling Resistive Synaptic Devices for Implementation of Unsupervised Learning with Spiking Neural Networks Yuhan Shi; University of California, San Diego, United States.

2:30 PM BREAK

SESSION EP06.03: Neuromorphic Devices II
Session Chairs: Xavier Obradors and Abu Sebastian
Tuesday Afternoon, April 3, 2018
PCC North, 200 Level, Room 221 C

3:30 PM *EP06.03.01

Neuromorphic Computing—Toward Dynamical Data Processing
Fabien Alibart^{1,2}; ¹IEMN-CNRS, France; ²LN2-CNRS, Canada.

4:00 PM EP06.03.02

Epitaxial Silicon-Germanium Artificial Synapses for Neuromorphic Computing Systems Scott H. Tan; Massachusetts Institute of Technology, United States.

4:15 PM EP06.03.03

Ferroelectric Coupled Oscillator Network for Neuromorphic Computing
Zheng Wang; Georgia Institute of Technology, United States.

4:30 PM *EP06.03.04

Dynamics, Design and Application of a Silicon-on-Insulator Technology Based Neuron Udayan Ganguly; IIT Bombay, India.

SESSION EP06.04: Poster Session
Tuesday Afternoon, April 3, 2018
5:00 PM - 7:00 PM
PCC North, 300 Level, Exhibit Hall C-E

EP06.04.01

Single- and Double-Gate Synaptic Transistors with a Reversible and Analog Drain Current Modulation Using a Pt/HfO_x/n-IGZO Memcapacitor Paul Yang; Myongji University, Korea (the Republic of).

EP06.04.02

Long- and Short-Term Potentiation and Depression in an Organic Electronic Synapse Jennifer Gerasimov; Linköping University, Sweden.

EP06.04.03

Artificial Synapse Based on Polymer-Blended Perovskite Sung Il Kim; Seoul National University, Korea (the Republic of).

EP06.04.04

Drift-Diffusion Simulation of Coupled Ionic-Electronic Devices
Steven McGarry; Carleton University, Canada.

EP06.04.05

Keystroke Dynamics Enabled Authentication and Identification Using Triboelectric Nanogenerator Array Changsheng Wu; Georgia Institute of Technology, United States.

EP06.04.06

Analog Memcapacitance Characteristics in Al/SiO₂/TaOx/n-IGZO Capacitor Structure for Synaptic Transistor Geon Won Beom; Myongji University, Korea (the Republic of).

EP06.04.07

Scaling Behaviour and Anatomy of Filamentary Threshold Switching in NbO_x Sanjoy K. Nandi; Australian National University, Australia.

EP06.04.08

A Synaptic Transistor Based on Two-Dimensional Molybdenum Oxide Dashan Shang; Institute of Physics, Chinese Academy of Sciences, China.

EP06.04.09

Polymer-Based Non-Volatile Analog Synapses for Low-Power Neuromorphic Computing Armantas Melianas; Stanford University, United States.

SESSION EP06.05: In-Memory Computing
Session Chairs: Bipin Rajendran and Abu Sebastian
Wednesday Morning, April 4, 2018
PCC North, 200 Level, Room 221 C

8:30 AM *EP06.05.01

Neuromorphic Computation for Hardware Acceleration of Deep Neural Networks—Challenges and Perspectives Geoffrey W. Burr; IBM Almaden Research Center, United States.

9:15 AM *EP06.05.02

Keynote: What is Beyond Deep and Narrow for AI? Dileep George; Vicarious AI, United States.

10:00 AM BREAK

10:30 AM *EP06.05.03

Keynote: Neural-Like Computing with Populations of Superparamagnetic Basis Functions Alice Mizrahi; National Institute of Standards and Technology, United States.

11:00 AM EP06.05.04

Flexible Ionic-Electronic Hybrid Oxide Synaptic TFTs with Programmable Dynamic Plasticity for Brain-Inspired Neuromorphic Computing
Rohit A. John^{1,4}; ¹Nanyang Technological University, Singapore; ⁴Nanyang Technological University, Singapore.

11:15 AM EP06.05.05

Increasing Information Storage Capacity in Computing Devices Formed from Self-Oscillating Gels Yan Fang; University of Pittsburgh, United States.

11:30 AM *EP06.05.06

Memristor-Based Analog Computations—Devices, Systems and Experimental Demonstrations Suhas Kumar; Hewlett Packard Labs, United States.

SESSION EP06.06: Materials and Devices for Large-Scale Data Analytics
Session Chairs: Geoffrey Burr and Manan Suri
Wednesday Afternoon, April 4, 2018
PCC North, 200 Level, Room 221 C

1:30 PM *EP06.06.01

Processing Big-Data with Metal-Oxide Memristors Themis Prodromakis^{1,2}; ¹University of Southampton, United Kingdom; ²Tsinghua University, China.

2:00 PM EP06.06.02

CMOS Compatible Temperature Anneal to Improve Artificial Synapses Based on HfO₂ ReRAM Devices Karsten Beckmann; SUNY Polytechnic Institute, United States.

2:15 PM EP06.06.03

Scalable Neuromorphic Computing Platform Based on Indium Phosphide Synaptic Device on Silicon Jun Tao; University of Southern California, United States.

2:30 PM BREAK

SESSION EP06.07: Computing Architectures Enabled by New Materials and Devices
Session Chairs: Suhas Kumar and Themis Prodromakis
Wednesday Afternoon, April 4, 2018
PCC North, 200 Level, Room 221 C

3:30 PM *EP06.07.01

Neuromorphic Architectures for Smart Sensing Applications—Lessons from the Insect Brain Angel Yanguas-Gil; Argonne National Laboratory, United States.

4:00 PM *EP06.07.02

Rewiring in Deep Neural Networks with Noisy Parameter Updates
Robert Legenstein; Graz University of Technology, Austria.

4:30 PM EP06.07.03

Organic Ferroelectric Memristors for Neuromorphic Computing
Sayani Majumdar; Aalto University, Finland.

4:45 PM EP06.07.04

Neuromorphic Computing by Organic Transistor Circuits
Paddy K. L. Chan; University of Hong Kong, Hong Kong.

SESSION EP06.08: Design and Modeling for Neuromorphic Computing
Session Chairs: Duygu Kuzum and Manan Suri
Thursday Morning, April 5, 2018
PCC North, 200 Level, Room 221 C

9:00 AM *EP06.08.01

Keynote: Transforming Nanodevices into NanoSystems—The N3XT 1,000X Subhasish Mitra; Stanford University, United States.

10:00 AM BREAK

10:30 AM *EP06.08.02

Design and CMOS Co-Integration of ReRAM Devices and Crossbar Arrays for Neuromorphic Applications Yusuf Leblebici; EPFL, Switzerland.

11:00 AM *EP06.08.03
Oxide Architectures and Defect Design for Next Materials in
Neuromorphic Computing [Jennifer L. Rupp](#); MIT, United States.

11:30 AM *EP06.08.04
Non-Volatile Memory Device Optimization Trends from *Ab Initio*
Simulations [Blanka Magyari-Kope](#); Stanford University, United States.

SESSION EP06.09: Neuromorphic Devices III
Session Chairs: Bipin Rajendran and Han Wang
Thursday Afternoon, April 5, 2018
PCC North, 200 Level, Room 221 C

1:30 PM *EP06.09.01
Analog HfO₂-Based Memristive Devices for Spiking Neural Networks
[Sabina Spiga](#); CNR-IMM, Italy.

2:00 PM EP06.09.02
Low-Power, Electrochemically-Tunable Graphene Synapses for
Neuromorphic Computing [Mohammad T. Sharbati](#); University of Pittsburgh,
United States.

2:15 PM EP06.09.03
Demonstrative Operation of Four-Terminal Memristive Devices by
Controlling Oxygen Vacancy Distribution in TiO_{2-x} Single Crystals
[Akira Sakai](#); Osaka University, Japan.

2:30 PM BREAK

SESSION EP06.10: Materials and Devices for Large Scale Computing Systems
Session Chairs: Yusuf Leblebici and Sabina Spiga
Thursday Afternoon, April 5, 2018
PCC North, 200 Level, Room 221 C

3:30 PM *EP06.10.01
Emerging 2D Material Devices for Neuromorphic Computing [Han Wang](#);
University of Southern California, United States.

4:00 PM EP06.10.02
Synaptic Learning and Memory Functions in Amorphous Yttria-Based
Memristive Systems [Mangal Das](#); Indian Institute of Technology, India.

4:15 PM EP06.10.03
Hybrid Synaptic Elements for Opto-Neuromorphic Computing
[Rohit A. John](#)^{1,2}; ¹Nanyang Technological University, Singapore; ²Nanyang
Technological University, Singapore.

4:30 PM EP06.10.04
Investigation of Resistive Switching Behavior for Glucose-Based
Biomaterials [Sung Pyo Park](#); Yonsei University, Korea (the Republic of).

4:45 PM EP06.10.05
Synaptic Functions Revealed in Dual Ion Beam Sputtered Zinc
Oxide Based Memristive Devices for Neuromorphic Computing
[Brajendra S. Sengar](#); IIT Indore, India.

SYMPOSIUM EP07

Phase-Change Materials and Their Applications—Memories,
Photonics, Displays and Non-von Neumann Computing
April 3 - April 5, 2018

Symposium Organizers

Harish Bhaskaran, University of Oxford
Kotaro Makino, National Institute of Advanced Industrial
Science and Technology
Stefania Privitera, CNR
Veronique Sousa, CEA LETI MINATEC

MRS Invitation to Publish

All authors are invited to submit articles based on their 2018 MRS Spring
Meeting presentations to journals in the MRS portfolio.
(www.mrs.org/publications-news) Papers submitted and accepted for
publication in MRS Advances (www.mrs.org/mrs-advances) will be
available as symposium collections. Visit the MRS/Cambridge University
Press Publications Booth #100 in the Exhibit Hall to learn more, including
MRS Advances print options available at special rates during the meeting
week only.

* Invited Paper

TUTORIAL

Phase-Change Materials—Basic Research to Industrial Applications

Monday Morning, April 2, 2018
PCC North, 200 Level, Room 222 A

8:00 AM – 9:30 AM
Part I: **Geoffrey W. Burr**
Memory Applications

Memory technology is rapidly evolving, as new nonvolatile memories (NVM) such as Phase Change Memory (PCM) and Resistive RAM (RRAM) emerge. Such memories have begun to enable Storage-Class Memory (SCM), by combining the high performance and robustness of solid-state memory with the long-term retention and low cost of conventional storage.

Simultaneously, as we seek to continue to improve computing systems, attention is turning to Non-Von Neumann algorithms, including computing architectures motivated by the human brain. The same large NVM arrays that have enabled initial SCM products can also be used in non-Von Neumann neuromorphic computational schemes, with device conductance serving as synaptic “weight.” This allows the all-important multiply-accumulate operation within these algorithms to be performed efficiently AT the weight data.

I will discuss these two broad classes of applications, and their various sub-classes. The sub-classes of SCM will include Memory-class SCM and Storage-class SCM applications; the sub-classes for Deep Learning Accelerators include Forward Inference-only applications (e.g., ex-situ training) and in-situ/on-chip Training. I will describe how the various application needs drive the target device specifications for the ideal PCM devices that would be needed to enable each of these applications.

9:30 AM – 10:00 AM BREAK

10:00 AM – 11:30 AM
Part II: **Hidekazu Tanaka**
Basics and Applications of Electronic Phase Change Oxides

Phase change materials enable rapid switching between different structural phases, resulting electric properties switching. Some classes of materials are interesting on switching between different electronic/spin phases itself, such as Mott insulator- metal transition, and their electronic phase change would produce new classes of devices. This part of the tutorial will focus on electronic phase change phenomena on transition metal oxides. Topics included will be:

Deformable Atomically-thin Materials – Mechanics, Materials and Devices

June 4, 2018

NM11 Lead Organizer: Dr. SungWoo Nam

- E-mail address : swnam@illinois.edu
- Institution : University of Illinois at Urbana-Champaign (UIUC)
- Mailing Address : 1206 W. Green St., MC-244, Urbana, IL 61801
- Phone : 1-217-300-0267
- Fax : 1-217-244-6534

Executive Summary:

Our NM11 symposium on Deformable Atomically-thin Materials – Mechanics, Materials and Devices was successfully held on April 2-6, 2018. Our symposium focused on disseminating and discussing research progress centered on how mechanical deformation of atomically-thin materials can be used to create functional morphologies for new materials properties and advanced device functions. Both invited and contributing speakers presented and discussed how surface morphologies and straining from deformable 2D materials systems can lead to unique and emerging physical and chemical functionalities. Our symposium attracted a sizable audience, averaging 60 attendees per presentation. With the support of ARO, we implemented NM11 Best Presentation Awards for students/postdocs (6 Gold Awards and 13 Silver Awards), with more than 20% of the recipients being women/minority students. We believe our symposium has led to the nucleation of new research direction/field of mechanically-coupled properties of 2D materials, and we expect that a similar symposium will be organized in future MRS Spring and Fall 2019 MRS Meetings.

Objectives:

Our NM11 symposium on April 2-6, 2018, entitled 'Deformable Atomically-thin Materials – Mechanics, Materials and Devices,' brought together researchers from academia, industry and government laboratories to engage in discussion on emerging areas of deformable atomically-thin materials. In particular, our symposium focused on how mechanical deformation of atomically-thin materials can be used to create functional morphologies for new materials properties and advanced device functions. Invited speakers from materials/chemistry, solid mechanics and device physics provided their expertise in their respective areas and initiated discussions on how we could further enhance/tailor materials properties by mechanical designs.

Presentations:

Our symposium had a total of 72 presentations with 22 invited speakers in the areas of synthesis, processing, mechanics, emerging physical/chemical properties, and device applications of deformable 2D materials. Our final talk schedule and abstracts are posted here:

https://mrsspring2018.zerista.com/event?owner_id=2011945&owner=other&event_order=start&event_page=1&tag_ids=397711

Highlights:

Invited presentations given by Professors Rodney Ruoff (UNIST) and Jiwoong Park (University of Chicago) (see photos below) on the synthesis of deformable atomically-thin materials on April 2, 2018 drew a peak number of attendees (>110 attendees).



Contributions to Discipline:

We believe our symposium has led to a nucleation of new research direction/field of mechanically-coupled properties of 2D materials, and we expect that similar symposiums will be organized in upcoming MRS Spring and Fall 2019 Meetings.

Future Direction of this Symposium Topic:

We expect that this area of research will continue to grow as there are emerging interests in Quantum Materials, Materials by Design and Soft Matter. The deformable electromechanical properties of atomically-thin materials will provide unique opportunities and promise in these emerging research areas. The lead organizer, Dr. SungWoo Nam, plans to be involved in several similar MRS symposiums in upcoming MRS Spring and Fall 2019 Meetings to build and strengthen the research community in this topic area.

A list of Those Supported with Grant Funds:

With the support of ARO, we were able to implement NM11 Best Presentation Awards for students/postdocs with 6 Gold Awards and 13 Silver Awards (>20% of the awards given to women/minority students). A list of awardees is included below. We are grateful for the generous grant support provided by ARO.

2018 MRS Spring Meeting NM11 Best Presentation Awards	
Gold (\$400)	
Name	Institution
Michelle Chen	Stanford University
Sabine M. Neumayer	Oak Ridge National Laboratory
Matthew R. Rosenberger	U.S. Naval Research Laboratory
Michael Cai Wang	University of Illinois at Urbana-Champaign
Saien Xie	Cornell University/University of Chicago
Keong Yong	University of Illinois at Urbana-Champaign
Silver (\$200)	
Name	Institution
Emil J. Annevelink	University of Illinois at Urbana-Champaign
Chullhee Cho	University of Illinois at Urbana-Champaign
Md Farhadul Haque	University of Illinois at Urbana-Champaign
Kyoung-Ho Kim	University of North Carolina at Chapel Hill
Anirudh Krishna	University of California, Irvine
Juyoung Leem	University of Illinois at Urbana-Champaign
Shuai Lou	University of California, Berkeley
Julian Ramirez	University of California, San Diego
Qun Su	University of Minnesota
Joonki Suh	University of Chicago
Wei Wu	University of Connecticut
Yiping Wang	Rensselaer Polytechnic Institute
Yuzhou Zhao	University of Wisconsin-Madison

SESSION NM10.12: Fundamental Deformation Mechanisms
Session Chairs: Michael Demkowicz and Erica Lilleodden
Thursday Afternoon, April 5, 2018
PCC North, 200 Level, Room 227 A

3:30 PM *NM10.12.01

Exploring the Plasticity and Hall-Petch Limit of Nanotwinned Silver by Microalloying [Frederic Sansoz](#); University of Vermont, United States.

4:00 PM NM10.12.02

Transition from Source- to Stress-Controlled Plasticity in Nanotwinned Materials Below a Softening Temperature [Seyedeh Mohadeseh Taheri Mousavi](#); Massachusetts Institute of Technology, United States.

4:15 PM *NM10.12.03

Deformation Mechanisms in Mg/Nb Based Nanolaminates [Irene J. Beyerlein](#); University of California, Santa Barbara, United States.

4:45 PM NM10.12.04

In Situ SEM and TEM Tensile Testing of Nanoporous Gold [Joshua Stuckner](#); Virginia Polytechnic Institute and State University, United States.

SESSION NM10.13: Poster Session II
Thursday Afternoon, April 5, 2018
5:00 PM - 7:00 PM
PCC North, 300 Level, Exhibit Hall C-E

NM10.13.01

A Ultra-Thin Cobalt Metal Film in Low-Temperature Photo-Assisted Atomic Layer Deposition [Zheng Y. Liang](#); National Tsing Hua University, Taiwan.

NM10.13.02

Accelerated Nano Super Bainite in Ductile Iron [Eric J. Zhao](#); Beijing New Oriental Foreign Language School at Yangzhou, China.

NM10.13.03

Tensile Behavior of Multilayer, Solid Solution and Phase Separated Cu-Co Films [Rohit Berlia](#); Arizona State University, United States.

NM10.13.04

The Processing-Structure-Property Relationship in High Strength, High Electrical Conductivity Al Matrix Calcium or Carbon Nanotube Reinforced Nanocomposites [Liang Tian](#)^{1,2}; ¹Iowa State University, United States; ²University of Central Florida, United States.

NM10.13.05

Fabrication of Multilayered Metal Sheet by Accumulative Roll Bonding Process [Hyoung-Wook Kim](#); Korea Institute of Materials Science, Korea (the Republic of).

NM10.13.06

Site-Selective Growth of Ag Nanocubes for Sharpening Their Corners and Edges, Followed by Elongation into Nanobars Through Symmetry Reduction [Shan Zhou](#); Georgia Institute of Technology, United States.

NM10.13.07

Effect of Sputter Pressure on Phase Formation, Texture and Stresses in Beta Ta Thin Films [Shefford P. Baker](#); Cornell University, United States.

NM10.13.08

Synthesis and Mechanical Behavior of a Freestanding, Nanocrystalline NiTi Film Under Cyclic Tensile Deformation [Paul Rasmussen](#); Arizona State University, United States.

NM10.13.09

Dealloyed Platinum-Bismuth Nanoparticles as High Activity Electrocatalysts for Dimethyl Ether Oxidation [Anastasios Angelopoulos](#); University of Cincinnati, United States.

SYMPOSIUM NM11

Deformable Atomically Thin Materials—Mechanics, Materials and Devices
April 2 - April 6, 2018

Symposium Organizers

Chi Hwan Li, Purdue University
SungWoo Nam, University of Illinois at Urbana-Champaign
Won Il Park, Hanyang University
Baoping Xu, University of Virginia

MRS Invitation to Publish

All authors are invited to submit articles based on their 2018 MRS Spring Meeting presentations to journals in the MRS portfolio. (www.mrs.org/publications-news) Papers submitted and accepted for publication in MRS Advances (www.mrs.org/mrs-advances) will be available as symposium collections. Visit the MRS/Cambridge University Press Publications Booth #100 in the Exhibit Hall to learn more, including MRS Advances print options available at special rates during the meeting week only.

* Invited Paper

SESSION NM11.01: Synthesis of Deformable 2D Materials I
Session Chairs: SungWoo Nam and Won Il Park
Monday Afternoon, April 2, 2018
PCC North, 200 Level, Room 226 C

1:30 PM *NM11.01.01

Novel 3D Structures of Graphene and Graphene Oxide [Rodney S. Ruoff](#)^{1,2}; ¹Ulsan National Institute of Science and Technology, Korea (the Republic of); ²IBS CMCM, Korea (the Republic of).

2:00 PM *NM11.01.02

3D Circuitry and Folding with 2D Crystals [Jiwoong Park](#); University of Chicago, United States.

2:30 PM NM11.01.03

Laser Processing of 2D Materials for Flexible Electronics [Nicholas Glavin](#); Air Force Research Laboratory, United States.

2:45 PM NM11.01.04

Strain-Engineered Growth of 2D Materials on Patterned Substrates [Kai Xia](#); Oak Ridge National Laboratory, United States.

3:00 PM BREAK

3:30 PM NM11.01.05

Ultrahard Carbon Film from Epitaxial Two-Layer Graphene [Angelo Bongiorno](#); College of Staten Island - CUNY, United States.

3:45 PM *NM11.01.06

Graphene and 2D Layered Materials—Device Application Prospect [Hyeon Jin Shin](#); Samsung Electronics, SAIT, Korea (the Republic of).

4:15 PM NM11.01.07

Non-Euclidean Atomically-Thin Crystals [Joonki Suh](#); University of Chicago, United States.

4:30 PM NM11.01.08

Strain-Engineered Atomically-Thin Superlattices with Lattice Coherence [Saen Xie](#)^{1,2}; ¹Cornell University, United States; ²The University of Chicago, United States.

SESSION NM11.02: Synthesis of Deformable 2D Materials II
Session Chair: Won Il Park
Tuesday Morning, April 3, 2018
PCC North, 200 Level, Room 226 C

10:30 AM *NM11.02.01

h-BN for 2D Electronics [Young Hee Lee](#)^{1,2}; ¹Sungkyunkwan University, Korea (the Republic of); ²Center for Integrated Nanostructure Physics, IBS, Korea (the Republic of).

11:00 AM NM11.02.02

Controllable Growth and Formation Mechanisms of Dislocated WS₂ Spirals [Yuzhou Zhao](#); University of Wisconsin-Madison, United States.

11:15 AM NM11.02.03

Simulation Guided Growth of 2D Materials—A Generalized Multiscale Framework Kasra Momeni^{1,2}; ¹Louisiana Tech University, United States; ²The Pennsylvania State University, United States.

11:30 AM NM11.02.04

Solution Based, Graphite Oxide Template Assisted Growth and Characterization of Large Scale, High-Temperature Stable Ultrathin Graphitic ZnO Kyle B. Tom^{1,2}; ¹University of California, Berkeley, United States; ²Lawrence Berkeley National Laboratory, United States.

11:45 AM NM11.02.05

Wrinkling of Graphene on Copper Dogukan Senyildiz; TOBB University of Economics and Technology, Turkey.

SESSION NM11.03: Synthesis of Deformable 2D Materials III

Session Chair: Baoxing Xu

Tuesday Afternoon, April 3, 2018

PCC North, 200 Level, Room 226 C

1:30 PM *NM11.03.01

Structure-Properties Relationship of Ultrafine Graphene Particles with Paper Ball-Like Shape Jiaxing Huang; Northwestern University, United States.

2:00 PM NM11.03.02

Facile Fabrication of Large-Area Atomically Thin Membranes by Bottom-Up Synthesis of Nanoporous Monolayer Graphene Piran Ravichandran Kidambi; Vanderbilt University, United States.

2:15 PM NM11.03.03

Novel Surface Molecular Functionalization Route to Enhance Environmental Stability of Tellurium Containing 2D Layers Sijie Yang; Arizona State University, United States.

2:30 PM BREAK

SESSION NM11.04: Mechanics of Deformable 2D Materials I

Session Chair: Baoxing Xu

Tuesday Afternoon, April 3, 2018

PCC North, 200 Level, Room 226 C

3:30 PM *NM11.04.01

Tuning Interlayer Coupling of van der Waals Materials with High Pressure Junjiao Wu; University of California, Berkeley, United States.

4:00 PM *NM11.04.02

Interface Mechanics and Its Effect on Morphology and Functions of 2D Nanomaterials Yong Zhu; North Carolina State University, United States.

4:30 PM *NM11.04.03

1D van der Waals Nano-Materials—Selenium and Tellurium Peide P. Ye; Purdue University, United States.

SESSION NM11.05: Mechanics of Deformable 2D Materials II

Session Chairs: SungWoo Nam and Baoxing Xu

Wednesday Morning, April 4, 2018

PCC North, 200 Level, Room 226 C

8:30 AM NM11.05.01

Universal Deformation Pathways and Flexural Hardening of Nanoscale 2D-Material Standing Folds Bernardo R. Neves; University Federal-Minas Gerais, Brazil.

8:45 AM NM11.05.02

Liquid Evaporation-Driven Deformation and Assembly Mechanics—From 2D Graphene to 3D Architected Structures Baoxing Xu; University of Virginia, United States.

9:00 AM *NM11.05.03

Mechanical Interactions at Interfaces of Atomically Thin Materials Rui Huang; The University of Texas at Austin, United States.

9:30 AM NM11.05.04

Strain and Edge/Interface Tailoring to Control 2H/1T' Phase Transition Songsong Zhou; University of Pennsylvania, United States.

9:45 AM NM11.05.05

Mechanical Properties of Ti₂C₂T_x MXene Alexey Lipatov; University of Nebraska – Lincoln, United States.

10:00 AM BREAK

10:30 AM *NM11.05.06

Moiré Patterns in 2D Materials Beyond Graphene—Van der Waals Dislocation Arrays Harley T. Johnson; University of Illinois at Urbana-Champaign, United States.

11:00 AM *NM11.05.07

A New Subcritical Nanostructure of Graphene—Crinkle-Ruga Structure and Its Novel Properties Kyung-Suk Kim; Brown University, United States.

11:30 AM NM11.05.08

Mechanical Properties of MXenes from *In Silico* Experiments Vadym Mochalin; Missouri University of Science and Technology, United States.

11:45 AM NM11.05.09

Multiscale Analysis of Grain Boundary Motion in Graphene Emil J. Annelink; University of Illinois at Urbana-Champaign, United States.

SESSION NM11.06: Mechanics of Deformable 2D Materials III

Session Chair: Baoxing Xu

Wednesday Afternoon, April 4, 2018

PCC North, 200 Level, Room 226 C

1:30 PM NM11.06.01

Chemically Derived Kirigami of Transition Metal Dichalcogenides Liang Cai^{1,2}; ¹University of Wisconsin-Madison, United States; ²University of Science and Technology of China, China.

1:45 PM NM11.06.02

Mechanically Robust Flexible Metal Electrodes by the Integration of Multi-Layer Graphene Chullhee Cho; University of Illinois at Urbana-Champaign, United States.

2:00 PM NM11.06.03

Strain Transfer Analysis of Encapsulated Atomically Thin Materials in Four-Point Bending Experiments Wei Wu; University of Connecticut, United States.

2:15 PM NM11.06.04

Negative Poisson's Ratio in Two-Dimensional Honeycomb Structures Guangzhao Qin; RWTH Aachen University, Germany.

2:30 PM BREAK

SESSION NM11.07: Mechanically Driven Processing of 2D Materials I

Session Chair: Chi Hwan Lee

Wednesday Afternoon, April 4, 2018

PCC North, 200 Level, Room 226 C

3:30 PM *NM11.07.01

Ultrathin, Transparent Silicon Nanomembranes—Properties and Applications Jong-Hyun Ahn; Yonsei University, Korea (the Republic of).

4:00 PM NM11.07.02

AFM “Squeegee” for the Creation of Clean 2D Material Interfaces Matthew R. Rosenberger; U.S. Naval Research Laboratory, United States.

4:15 PM NM11.07.03

Fabrication and Surface Engineering of Two-Dimensional SnS Toward Piezoelectric Nanogenerator Application Naoki Higashitarumizu; The University of Tokyo, Japan.

SESSION NM11.08: Poster Session: Deformable 2D Materials I

Session Chair: SungWoo Nam

Wednesday Afternoon, April 4, 2018

5:00 PM - 7:00 PM

PCC North, 300 Level, Exhibit Hall C-E

NM11.08.01

3D Architecture Based on 2D Lateral Heterojunction Shuai Lou; University of California, Berkeley, United States.

NM11.08.02

Insights on Mechanical Properties of WS₂/MoS₂ Heterostructures Ygor M. Jaques; University of Campinas, Brazil.

NM11.08.03

A Self-Sacrificing Camphor-Assisted Clean Transfer of Graphene Nianduo Cai; Southern University of Science and Technology, China.

NM11.08.04

Large Area Photonic Crystallization of 2D MoS₂ for Flexible Electronics Richard H. Kim; Wright-Patterson Air Force Research Laboratory, United States.

NM11.08.05

Optimization of Graphene Mesh and Silicon Schottky-Junction by External Field-Effect for High Efficiency Solar Cells Su Han Kim; Hanyang University, Korea (the Republic of).

NM11.08.06

Non-Contact Flow and Particle Measurements via Elastohydrodynamic Deformation with Graphene Nano-Island Sensors Charles Dhong; University of California, San Diego, United States.

SESSION NM11.09: Mechanically Driven Processing of 2D Materials II
Session Chairs: Chi Hwan Lee and SungWoo Nam
Thursday Morning, April 5, 2018
PCC North, 200 Level, Room 226 C

8:00 AM NM11.09.01

Quantifying Disorder in CVD Graphene Induced by Ripples from Thermal Expansion Mismatch Qun Su; University of Minnesota, United States.

8:15 AM NM11.09.02

0D/1D/2D Meta-Materials—Large-Scale, Highly-Ordered Self-Assembly of 0D/1D Plasmonic Nanoparticle Arrays on Deterministically Deformed Monolayer 2D Materials Templates Michael Cai Wang; University of Illinois-Urbana-Champaign, United States.

8:30 AM *NM11.09.03

Multi-Scale Patterning of Conformable Deformable Thin Materials Teri W. Odom; Northwestern University, United States.

9:00 AM *NM11.09.04

Active Origami with 2D Materials Paul McEuen; Cornell University, United States.

9:30 AM NM11.09.05

Experimental Exploration of High Mobility Metal Phosphides—Vapor Phase Deposition of Two-Dimensional SiP Yiping Wang; Rensselaer Polytechnic Institute, United States.

9:45 AM BREAK**10:15 AM *NM11.09.06**

Strain Engineering of 2D Materials Teng Li; University of Maryland, College Park, United States.

10:45 AM *NM11.09.07

Continuously Tunable Uniaxial Strain Engineering in Graphene via Self-Rolled-Up Membrane Technology Xiuling Li; University of Illinois at Urbana-Champaign, United States.

11:15 AM NM11.09.08

Surface Acoustic Wave Exfoliation of Piezoelectric Stratified MoS₂ Md Mohiuddin; RMIT University, Australia.

11:30 AM NM11.09.09

Kirigami-Inspired Strain-Independent Functional Graphene Devices Kcong Yong; University of Illinois Urbana-Champaign, United States.

SESSION NM11.10: Emergent Properties of Deformable 2D Materials I
Session Chairs: Chi Hwan Lee and SungWoo Nam
Thursday Afternoon, April 5, 2018
PCC North, 200 Level, Room 226 C

1:30 PM *NM11.10.01

Ballistic Thermal Transport in Two-Dimensional MoSe₂ Lattices Adrian Bachtold; ICFO, Spain.

2:00 PM *NM11.10.02

MoS₂-Based Nanoelectromechanics Andras Kis; Ecole Polytechnique Federale de Lausanne, Switzerland.

2:30 PM BREAK**3:30 PM *NM11.10.03**

Novel Nanophotonic Devices—Graphene-Based Nanolasers and Photon-Triggered Nanowire Transistors Hong-Gyu Park; Korea University, Korea (the Republic of).

4:00 PM *NM11.10.04

Nanomaterial-Based Strain Sensors for Space Applications Mahmooda Sultana; NASA Goddard Space Flight Center, United States.

4:30 PM NM11.10.05

Giant Negative Electrostriction and Dielectric Tunability in a van der Waals Layered Ferroelectric Sabine M. Neumayer; University College Dublin, Ireland.

SESSION NM11.11: Poster Session: Deformable 2D Materials II
Session Chair: SungWoo Nam
Thursday Afternoon, April 5, 2018
5:00 PM - 7:00 PM
PCC North, 300 Level, Exhibit Hall C-E

NM11.11.02

Size and Strain-Induced Tuning of Properties of MoS₂ Nanostructures Shubham Bhagat; Guru Nanak Dev University, India.

NM11.11.03

Friction for Polycrystalline Graphene on Flexible Substrates as Transparent Flexible Sensors Qing Yu; Sinosteel Corporation Wuhan Safety & Environmental Protection Research Institute, China.

NM11.11.04

Investigated NTC Semiconductor Nano-Particles and Graphene Flexible Hybrid Material as Multiple-Role Sensor Lihong Su; Northwest Polytech University, China.

NM11.11.05

Topography Induced Tunable Flexoelectricity in Mono-Layer MoS₂ Md Farhadul Haque; University of Illinois at Urbana-Champaign, United States.

NM11.11.06

The Internal Buckling Behavior Induced by Growth Self-Restriction in Vertical Multi-Walled Carbon Nanotube Arrays Guoan Cheng; Beijing Normal University, China.

SESSION NM11.12: Emergent Properties of Deformable 2D Materials II and Deformable 2D Electronics I
Session Chair: Pilgyu Kang
Friday Morning, April 6, 2018
PCC North, 200 Level, Room 226 C

8:30 AM NM11.12.01

Vertical Field-Effect Transistor Using ZnO Nanotubes Grown on Graphene Films for Flexible Inorganic Electronics Hongseok Oh^{1,2,3}; ¹Seoul National University, Korea (the Republic of); ²Seoul National University, Korea (the Republic of); ³Seoul National University, Korea (the Republic of).

8:45 AM NM11.12.02

Electrostatic Cycling of Suspended Graphene Thermal Switches Michelle Chen; Stanford University, United States.

9:00 AM *NM11.12.03

Soft Curved Image Sensor Array Using MoS₂ and Graphene Dae-Hyeong Kim^{2,1}; ¹Seoul National University, Korea (the Republic of); ²Institute for Basic Science, Korea (the Republic of).

9:30 AM NM11.12.04

Role of Surface Induced Defect States on Thermoelectric Power Factor in MoS₂ Manjunath C. Rajagopal; University of Illinois at Urbana-Champaign, United States.

9:45 AM NM11.12.05

Defect Mediated Molecular Interaction and Charge Transfer in Graphene-Based Electrolyte-Gated FET Sensors Sun Sang Kwon; Hanyang University, Korea (the Republic of).

10:00 AM BREAK

SESSION NM11.13: Deformable 2D Electronics II
Session Chair: Won Il Park
Friday Morning, April 6, 2018
PCC North, 200 Level, Room 226 C

10:30 AM *NM11.13.01
Mechanics and Functionalities of Graphene Electronic Tattoos (GETs)
Nanshu Lu; University of Texas at Austin, United States.

11:00 AM NM11.13.02
Excitation of Plasmonic Waves in Curved Graphene Nanostructures by Subwavelength Periodic Modulation Kyoung-Ho Kim; University of North Carolina at Chapel Hill, United States.

11:15 AM NM11.13.03
Fabrication of Graphene Oxide/Graphene Vertical Heterostructure Film and Its Use in Flexible Organic Light Emitting Diodes Jinhong Du; Institute of Metal Research, Chinese Academy of Sciences, China.

11:30 AM NM11.13.04
Crumple Nanostructuring of Atomically Thin Materials for High Performance Devices Pilgyu Kang; George Mason University, United States.

11:45 AM NM11.13.05
Ultrasensitive and Stretchable Graphene Electrodes Nan Liu^{1,2}; ¹Beijing Normal University, China; ²Stanford University, United States.

SESSION NM11.14: Deformable 2D Electronics III
Session Chair: Won Il Park
Friday Afternoon, April 6, 2018
PCC North, 200 Level, Room 226 C

1:30 PM NM11.14.01
Thin, Needle-Based Piezoelectric Systems for Guided Tissue Targeting by Mechanical Sensing Xinge Yu^{1,2}; ¹Northwestern University, United States; ²University of Illinois at Urbana-Champaign, United States.

1:45 PM NM11.14.02
Metallic Nanoislands on Graphene and Machine Learning for Monitoring Swallowing Activity in Head and Neck Cancer Patients Julian Ramirez; University of California San Diego, United States.

2:00 PM NM11.14.03
Mechanically Crumpled Two-Dimensional Semiconductor for Enhanced Photosensitivity Juyoung Leem; University of Illinois at Urbana Champaign, United States.

2:15 PM NM11.14.04
Bio-Inspired Radiative Cooling and Reconfigurable Surface Emissivity of Crumpled Graphene Anirudh Krishna; University of California, Irvine, United States.

SYMPOSIUM NM12

Transitioning Quantum Dots from Benchtop to Industry
April 3 - April 5, 2018

Symposium Organizers

Wan Ki Bae, Korea Institute of Science and Technology
Brian Korgel, University of Texas at Austin
Hunter McDaniel, UbiQD, LLC
Lazaro Padilha, Universidade Estadual de Campinas

Symposium Support UbiQD, Inc.

MRS Invitation to Publish

All authors are invited to submit articles based on their 2018 MRS Spring Meeting presentations to journals in the MRS portfolio. (www.mrs.org/publications-news) Papers submitted and accepted for publication in MRS Advances (www.mrs.org/mrs-advances) will be available as symposium collections. Visit the MRS/Cambridge University Press Publications Booth #100 in the Exhibit Hall to learn more, including MRS Advances print options available at special rates during the meeting week only.

* Invited Paper

SESSIONNM12.01: QD Photodetectors
Session Chairs: Hunter McDaniel and Lazaro Padilha
Tuesday Morning, April 3, 2018
PCC North, 200 Level, Room 228 A

10:30 AM *NM12.01.01
Colloidal Quantum Dots for Mid-Infrared Applications Philippe Guyot-Sionnest; University of Chicago, United States.

11:00 AM NM12.01.02
Near-Infrared Optoelectronics Using HgTe Colloidal Quantum Wells Clement Livache^{1,2}; ¹ESPCL, France; ²Université Pierre et Marie Curie, France.

11:15 AM *NM12.01.03
Direct Casting of Conductive Lead Chalcogenide Nanocrystal Films—Turning Ligands from Foe to Friend Jeffrey M. Pietryga; Los Alamos National Laboratory, United States.

11:45 AM NM12.01.04
Probing the Energy Landscape of PbS QDs via Capacitance Spectroscopy Eric Wong; University of Pennsylvania, United States.

SESSION NM12.02: QD Products and Manufacturing
Session Chairs: Doh Lee and Jeffrey Pietryga
Tuesday Afternoon, April 3, 2018
PCC North, 200 Level, Room 228 A

1:30 PM *NM12.02.01
Development of Heavy Metal-Free Quantum Dots—From Lab Bench to Commercial Applications Nigel L. Pickett; Nanoco Technologies Limited, United Kingdom.

2:00 PM NM12.02.02
Upscaling Colloidal Nanocrystal Hot-Injection Syntheses via Reactor Underpressure Maksym Yarema; ETH Zurich, Switzerland.

2:15 PM NM12.02.03
Toward a Thermodynamic Profile for Cadmium-Based Quantum Dot Surface Chemistry via Isothermal Titration Calorimetry Megan Y. Gee; University of South Carolina, United States.

2:30 PM BREAK

3:30 PM *NM12.02.04
From Quantum Dots to Holography Seth Coe-Sullivan; Luminit, LLC, United States.

4:00 PM NM12.02.05
Correlated Atomic Structure and Single Nanocrystal Photophysics for Directed Colloidal Quantum Dot Synthesis James R. McBride; Vanderbilt University, United States.