

# CENTER FOR INTEGRATED NANOTECHNOLOGIES ANNUAL MEETING

PROGRAM

Sept 22-24 2019 Santa Fe, NM

#### CODE OF CONDUCT

The 2019 CINT Annual Meeting is dedicated to providing a harassment-free conference experience for everyone, regardless of gender, gender identity and expression, sexual orientation, disability, physical appearance, body size, race, age, or religion. We do not tolerate harassment of conference participants in any form. Creating a supportive environment to enable scientific discourse at CINT events is the responsibility of all participants. Conference participants violating these rules may be sanctioned or expelled from the conference without a refund at the discretion of the conference organizers.

If you are being harassed, notice that someone else is being harassed, or have any other concerns, please contact one of the conference organizers at the registration table immediately.

Conference organizers, and any CINT staff member, will be happy to help participants contact hotel security or local law enforcement, provide escorts, or otherwise assist those experiencing harassment to feel safe for the duration of the conference. We value your attendance.

#### 2019 CINT ANNUAL MEETING SYMPOSIA



#### September 22-24, 2019

La Fonda on the Plaza Santa Fe, NM

#### **Computation and Theory of Soft Matter**

September 22-24, 2019 New Mexico Room, Stiha Room Organizers: Dvora Perahia, Lisa Hall, Gary Grest

The Computation and Theory of Soft Matter Symposium aims to bring together scientists to discuss recent developments in theory and modeling of soft matter nanomaterials.

#### Machine Learning for Nanoscale Materials Joint NSRC Symposium

September 23-24, 2019 New Mexico Room Organizers: Mark Stevens, Rémi Dingreville, Rajiv Kalia, Ryan Wixom

The Machine Learning for Nanoscale Materials Symposium will address how machine learning can be applied to nanoscale materials by bringing together experts from all five of the Nanoscale Science Research Centers and experts in quantum materials, nanophotonics, soft matter, and characterization.

#### **2D Materials**

September 23-24, 2019 Ballroom South Organizers: Rohit Prasankumar, Jinkyoung Yoo, Ekaterina Dolgopolova, Jennifer Hollingsworth

The 2D Materials Symposium will bring together experts in the characterization and fabrication of 2D materials, including multi-dimensional hybrid structures, van der Waals heterostructures, and non-traditional 2D materials, to foster new scientific directions in this exciting field.



### **CINT Annual Meeting**

#### September 22-24, 2019

#### La Fonda on the Plaza, Santa Fe, New Mexico



#### Sunday Morning, September 22

| 8:00 am   | Registration                                                                                                                                          |                 | Mezzanine |
|-----------|-------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------|-----------|
| Symposium | Computation and Theory<br>of Soft Matter                                                                                                              |                 |           |
|           | New Mexico Room                                                                                                                                       |                 |           |
|           | <b>Moderators:</b><br>Gary Grest, Lisa Hall                                                                                                           |                 |           |
| 9:00 am   | Phil Pincus<br>University of California, Santa Barbara<br>"Polyelectrolyte Persistence Length Revisited"                                              |                 |           |
| 9:30 am   | Mark Stevens<br>CINT<br>"Recent Results in Polyelectrolyte Simulations"                                                                               |                 |           |
| 10:00 am  | <b>Bobby Sumpter</b><br>Center for Nanophase Materials Sciences (ORNL)<br><i>"Understanding and Tailoring Transport in Polymerized Ionic Liquids"</i> |                 |           |
| 10:30 am  | Break                                                                                                                                                 |                 |           |
| 10:50 am  | <b>Cynthia Olson Reichhardt</b><br>Los Alamos National Laboratory<br><i>"Crossover from jamming to clogging in disordered environments"</i>           |                 |           |
| 11:20 am  | Ishan Srivastava<br>Sandia National Laboratories<br>"Statistics and Rheology of Granular Materials at the Flow-Arrest Transition"                     |                 |           |
| 11:50 am  | Jeremey Lechman<br>Sandia National Laboratories<br>"Modeling Particle Mechanics in Fine Powders"                                                      |                 |           |
| 12:20 pm  | Lunch Break<br>Please enjoy lunch at the café in the hotel or numerous restaurants surro                                                              | ounding the pla | ıza.      |

#### Sunday Afternoon, September 22

| Symposium         | Computation and Theory                                                                                                                                  |    |               |
|-------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------|----|---------------|
|                   | of Soft Matter                                                                                                                                          |    |               |
|                   | New Mexico Room                                                                                                                                         |    |               |
|                   | <i>Moderators:</i><br>Dvora Perahia, Michael Rubinstein                                                                                                 |    |               |
| 1:20 pm           | <b>Lisa Hall</b><br>Ohio State University<br>"Analyzing Ion Conductivity of Polymer Electrolytes from Coarse-Grained<br>Molecular Dynamics Simulations" |    |               |
| 1:50 pm           | Sidath Wijesinghe<br>Clemson University and University of North Carolina<br>"Soft nanoparticles at the interface of bio membranes"                      |    |               |
| 2:20 pm           | <b>Dipak Aryal</b><br>University of Texas<br>"Transport of Water in Polymer Membranes: Computational Studies"                                           |    |               |
| 2:50 pm           | Break                                                                                                                                                   |    |               |
| 3:10 pm           | <b>Steve Plimpton</b><br>Sandia National Laboratories<br>"Accelerated Molecular Dynamics for Rare-Event Systems via the<br>Hyperdynamics Method"        |    |               |
| 3:40 pm           | <b>Mesfin Tsige</b><br>University of Akron<br>"Dynamics of Interfacial Water via Instantaneous Water/Polymer Interfaces"                                |    |               |
| 4:10 pm           | <b>Dvora Perahia</b><br>Clemson University<br><i>"From Molecule to Membrane: Structured Ionic Polymers"</i>                                             |    |               |
| 4:40 pm           | End of daily session                                                                                                                                    |    |               |
| 5:30 pm           | Evening reception<br>hors d'oeuvres & cash bar<br>Pre-registration required                                                                             | Ba | allroom North |
| 6:30 –<br>8:00 pm | No Host Dinner<br>Pre-registration required                                                                                                             | Ba | allroom North |

#### Monday Morning, September 23

| 7:30 am  | Registration                                                                   | Mezzanine                  |
|----------|--------------------------------------------------------------------------------|----------------------------|
|          | Continental Breakfast                                                          | Ballroom North             |
| 8:45 am  | Plenary Session                                                                | Ballroom South             |
|          | Welcome                                                                        |                            |
|          | Antoinette Taylor, Associate Laboratory Director, Physical Sciences, Los Alamo | os National Laboratory     |
|          | Grant Heffelfinger, Deputy Chief Research Officer and Director of Advanced Sc  | ience & Technology, Sandia |
|          | National Laboratories                                                          |                            |
| 9:00 am  | NSRC Update                                                                    |                            |
|          | George Maracas, Program Manager Nanoscale Science Research Centers, Offic      | e of Basic Energy Sciences |
| 9:10 am  | Introductions, CINT Update and CINT User Recognition Award                     |                            |
|          | Jeff Nelson, CINT Director and Ross McDonald, CINT Co-Director (acting)        |                            |
| 9:30 am  | Prof. Tony F. Heinz                                                            | Ballroom South             |
|          | Stanford University                                                            |                            |
|          | "Probing and controlling excitons in 2D materials and heterostructures"        |                            |
| 10:10 am | Break                                                                          |                            |
| 10:30am  | Prof. Timothy P. Lodge                                                         | Ballroom South             |
|          | University of Minnesota                                                        |                            |
|          | "Bicontinuous Structures in Charged Polymer Materials"                         |                            |
| 11:10 am | Prof. Rajiv Kalia                                                              | Ballroom South             |
|          | University of Southern California                                              |                            |
|          | "Deep Learning in Nanoscience"                                                 |                            |
| 11:50 am | Working lunch and poster review                                                | Ballroom North             |
|          |                                                                                |                            |
| 12:00 pm | UEC Sponsored working lunch:                                                   | Ballroom South             |
| •        | "Presentation Zen: Let's free ourselves from bad PowerPoint"                   | (Please pick up your lunch |
|          | Guest speaker: Ryan Wixom                                                      | from Ballroom North and    |
|          |                                                                                | bring to Ballroom South)   |

#### Monday afternoon, September 23

| 2019 CINT Annual Meeting – Parallel Symposia |                                                                                                         |                                                                                                             |                                                                                                                                                                                              |
|----------------------------------------------|---------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Symposia                                     | Computation and Theory<br>of Soft Matter                                                                | 2D Materials                                                                                                | Machine Learning for<br>Nanoscale Materials                                                                                                                                                  |
|                                              | Stiha Room                                                                                              | Ballroom South                                                                                              | New Mexico Room                                                                                                                                                                              |
|                                              | <b>Moderators:</b><br>Mesfin Tsige, Phil Pincus                                                         | <b>Moderators:</b><br>Rohit Prasankumar, Jinkyoung Yoo,<br>Ekaterina Dolgopolova, Jennifer<br>Hollingsworth | <b>Moderators:</b><br>Mark Stevens, Rajiv Kalia, Rémi<br>Dingreville, Ryan Wixom                                                                                                             |
| 1:15 pm                                      | <b>Sanat Kumar</b><br>Columbia University<br>"Polymer Grafted Nanoparticle<br>Gas-Separation Membranes" | <b>Prof. Jim Schuck</b><br>Columbia University<br>"Nano and nonlinear photonics in<br>2D semiconductors"    | Rama Vasudevan<br>Center for Nanophase<br>Materials Sciences (ORNL)<br>"Deep and machine learning for<br>materials: Accelerating<br>imaging, synthesis, and physics<br>knowledge generation" |

| 1:45 pm              | Shengfeng Cheng                                                                                                                                                                                                                                                              | Elaine Li                                                                                                                                                                     | Steve Whitelam                                                                                                                                           |
|----------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------|
|                      | Virginia Tech<br>"Drying of Soft Matter Solutions"                                                                                                                                                                                                                           | University of Texas at Austin<br>"Moire Excitons in van der Waals<br>Heterostructures"                                                                                        | The Molecular Foundry (LBL)<br>"Playing games of physics:<br>evolutionary reinforcement<br>learning to extremize path-<br>extensive physical quantities" |
| 2:15 pm              | <b>Ting Ge</b><br>Duke University<br>"Mobility of Polymer-Tethered<br>Nanoparticles in Unentangled<br>Polymer Melts."                                                                                                                                                        | Libai Huang<br>Purdue University<br>"Spatial and temporal imaging of<br>exciton transport in 2D<br>heterostructures"                                                          | <b>Pankaj Rajak</b><br>Argonne National Laboratory<br>"Generative and Reinforcement<br>Learning for Interfaces and<br>Metamaterial Design"               |
| 2:45 pm              | Amalie Frischknecht<br>CINT<br>"Assembly of Polymer-Grafted<br>Nanoparticles"                                                                                                                                                                                                | <b>David Reis</b><br>Stanford University<br><i>"High-harmonic generation in</i><br><i>nanoscale and 2D materials"</i>                                                         | Mathew Cherukara<br>Center for Nanoscale Materials<br>(ANL)<br>"Real-time 3D nanoscale<br>imaging via deep learning and<br>automatic differentiation"    |
| 3:15 pm              | Break                                                                                                                                                                                                                                                                        | Break                                                                                                                                                                         | Break                                                                                                                                                    |
| 3:35 pm              | Jonathan Bollinger<br>Sandia National Laboratories<br>"Shape change as a driving force<br>for the dynamic instability of<br>microtubules"                                                                                                                                    | <b>Chenfeng Ke</b><br>Dartmouth College<br><i>"Hierarchical Co-Assembly</i><br><i>Enhanced Direct Ink Writing of 2D</i><br><i>and 3D Materials"</i>                           | <b>Sergei Tretiak</b><br>CINT<br>"Machine Learning for Chemical<br>Properties and Materials"                                                             |
| 4:05 pm              | J. Matthew Lane<br>Sandia National Laboratories<br>"Nanoparticles under Pressure:<br>Dynamic Assembly and Phase<br>Transition Modeling and<br>Experiments"                                                                                                                   | Katherine Mirica<br>Dartmouth College<br>"Molecular Engineering of<br>Multifunctional 2D Framework<br>Materials"                                                              | <b>Trevor Rhone</b><br>Rensselaer Polytechnic<br>Institute<br><i>"Machine learning study</i><br><i>magnetic of van der Waals</i><br><i>materials"</i>    |
| 4:35 pm              | Edmund Webb III<br>Lehigh University<br>"Multiscale Modeling of<br>Macromolecular Proteins in<br>Human Blood Flow"                                                                                                                                                           | Nathan Flanders (on behalf of<br>Prof. William Dichtel)<br>Northwestern University<br>"In situ observation of the<br>nucleation and growth of covalent<br>organic frameworks" | Willie Padilla<br>Duke University<br>"Deep learning for accelerated<br>all-dielectric metasurface<br>design"                                             |
| 4:55pm               | End of daily session                                                                                                                                                                                                                                                         | Wanyi Nie<br>CINT<br>"Two-dimensional hybrid<br>perovskite materials<br>semiconductors: Structure and<br>opto-electronic properties"                                          | Jacob Taylor<br>University of Maryland<br>"Machine learning for<br>automated formation of<br>quantum dot arrays"                                         |
| 5:15 pm -<br>7:00 pm | Poster Session and light dinner will be held on the La Terraza Terrace1 Drink ticket per attendee provided courtesy of our sponsors.Tickets will be handed out at the start of the poster session.CINT User Recognition Award poster, Prof. Haiyan Wang (Purdue University): |                                                                                                                                                                               |                                                                                                                                                          |
|                      | "Metal-ceramic nanocomposite thin                                                                                                                                                                                                                                            | film: Towards tunable 3D structures a                                                                                                                                         | nd multi-functionalities"                                                                                                                                |

#### Tuesday Morning. September 24

| 7:30 am                                                      | Registration<br>Continental Breakfast                                                                                                                                                                           |                                                                                                                                                                                        | Mezzanine<br>Ballroom North                                                                                                                                                          |  |
|--------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--|
|                                                              | Plenary Session                                                                                                                                                                                                 |                                                                                                                                                                                        |                                                                                                                                                                                      |  |
| 8:30 am                                                      | <b>Prof. Chad A. Mirkin</b><br>Northwestern University<br><i>"Expanding and Exploring the Mater</i>                                                                                                             | <b>Ballroom South</b><br>rials Genome Through Cantilever-Free Scanning Probe Lithography"                                                                                              |                                                                                                                                                                                      |  |
| SymposiaComputation and Theory<br>of Soft Matter2D Materials |                                                                                                                                                                                                                 | 2D Materials                                                                                                                                                                           | Machine Learning for<br>Nanoscale Materials                                                                                                                                          |  |
|                                                              | Stiha Room                                                                                                                                                                                                      | Ballroom South                                                                                                                                                                         | New Mexico Room                                                                                                                                                                      |  |
|                                                              | <i>Moderators:</i><br>Shengfeng Cheng, Sanat Kumar                                                                                                                                                              | <b>Moderators:</b><br>Rohit Prasankumar, Jinkyoung<br>Yoo, Ekaterina Dolgopolova,<br>Jennifer Hollingsworth                                                                            | <b>Moderators:</b><br>Mark Stevens, Rajiv Kalia, Rémi<br>Dingreville, Ryan Wixom                                                                                                     |  |
| 9:15 am                                                      | Marco A. Galvani Cunha and<br>Mark O. Robbin<br>Johns Hopkins University<br>"Effect of Chain Alignment on<br>Entanglements, Diffusion,<br>Relaxation and Polymer Weld<br>Strength in Additive<br>Manufacturing" | Maxim Sukharev<br>Arizona State University<br>"Optics of exciton-plasmon<br>nanostructures"                                                                                            | Mark Hybertsen<br>Center for Functional<br>Nanomaterials (BNL)<br>"Predicting local atomic<br>structures from X-ray absorption<br>spectroscopy using theory and<br>machine learning" |  |
| 9:45 am                                                      | <b>K. Michael Salerno</b><br>US Army Research Laboratory<br>"Modeling Soft Materials and<br>Interfaces Using Atomistic and<br>Coarse Grained Models"                                                            | <b>Pinshane Huang</b><br>University of Illinois at Urbana-<br>Champaign<br>"Characterizing unconventional<br>strain and bending in 2D<br>materials with aberration-<br>corrected STEM" | Jeffery Aguiar<br>Idaho National Laboratory<br>"Coding in the (Potential) Great<br>Leaps in Multidimensional<br>Microscopy and Materials<br>Discovery"                               |  |
| 10:15 am                                                     | Break                                                                                                                                                                                                           | Break                                                                                                                                                                                  | Break                                                                                                                                                                                |  |
| 10:35 am                                                     | <b>Thomas O'Connor</b><br>Sandia National Laboratories<br>"Simulating the Far from<br>Equilibrium Dynamics & Rheology<br>of Elongated Polymer"                                                                  | Wei Kong<br>Massachusetts Institute of<br>Technology<br>"Opportunity and challenges in 2D<br>material-based layer transfer<br>(2DLT) of III-N system"                                  | <b>Debra Audus</b><br>National Institute of Standards<br>and Technology (NIST)<br><i>"Enabling polymer informatics</i><br><i>through databases"</i>                                  |  |
| 11:05 am                                                     | Michael Rubinstein<br>Duke University<br>"Shear and Extensional Flow of<br>Ring Polymer Melts"                                                                                                                  | Chang-yong Nam<br>Center for Functional<br>Nanomaterials (BNL)<br>"2D heterostructure Research at<br>the Center for Functional<br>Nanomaterials"                                       | Panel Discussion                                                                                                                                                                     |  |

| 11:35 pm | <b>Gary Grest</b><br>CINT<br>"Molecular Simulations of<br>Entangled Polymers"         | Taisuke OhtaCINT"Probing atomic arrangement andelectronic band alignment of 2Dmaterials using surface electronmicroscopy" | Panel Discussion                                                                      |
|----------|---------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
| 12:05 pm | <b>Concluding Remarks by</b><br><b>Symposium Organizer</b><br>****End of Symposium*** | <b>Concluding Remarks by</b><br><b>Symposium Organizer</b><br>****End of Symposium***                                     | <b>Concluding Remarks by</b><br><b>Symposium Organizer</b><br>****End of Symposium*** |
| 12:05 pm | Working lunch & poster review                                                         |                                                                                                                           | Ballroom North                                                                        |
| 12:05pm  | <i>User Executive Committee lunch meeting &amp; photo (closed session)</i>            |                                                                                                                           | Ballroom South                                                                        |
| 1:00 pm  | NSRC AI/ML Meeting<br>(closed session)                                                |                                                                                                                           | Stiha Room                                                                            |

# Thank you to our sponsors for supporting the CINT Annual Meeting and our community of users.





- PROF. TONY HEINZ -

Stanford University

#### Monday, September 23, 2019 | 9:30am

La Fonda on the Plaza Ballroom South

#### Probing and Controlling Excitons in 2D Semiconductors and Heterostructures

In 2D semiconductors, the reduced dimensionality and reduced dielectric screening causes many-body interactions to play a central role in the materials' electronic and optical properties. As a consequence, excitons dominate the optical excitations. Here, we describe advances in understanding the excitonic properties of 2D semiconductors consisting of monolayers in the transition metal dichalcogenide (TMDC) family of MX2 (M = Mo, W; X = S, Se, Te). In this paper, we describe recent advances in the spectroscopy of TMDC semiconductors through the use of stacking of layered materials. By preparing a heterostructure encapsulated in h-BN and arranged with electrical gating, we have gained a much more comprehensive picture of the various excitonic states supported in these materials. In particular, such encapsulated WSe2 monolayers exhibit emission features with meV-wide features, allowing us to observe, 2-, 3-, 4-, and 5- body excitonic complexes in spin-allowed and spinforbidden configurations. We will also describe how the surrounding media alter the electronic structure of the encapsulated monolayer and how this can be used to deliberately alter the electrical and optical gaps of the semiconductor. Stacking two different monolayers with different band-gaps gives rise to the possibility of charge separation and the formation of interlayer excitons after optical excitation. We will present recent results on a new method to monitor the rapid charge separation using the associated of emission of THz radiation. At the same time, the final state resulting from charge transfer is directly observable through the emission of interlayer exciton states. In this context, we describe the interlayer exciton in the MoS2/WSe2 heterostructure. We find that the lowest-lying interlayer exciton has an energy around 1 eV, which can be tuned by more than 100 meV using electrical gating. In addition to providing fundamental understanding of this system, our results suggest the availability of broadly and readily tunable light sources based on 2D semiconductor heterostructures.



**Prof. Tony Heinz** is Professor of Applied Physics and Photon Science at Stanford University and the Director of the Chemical Sciences Division at the SLAC National Accelerator Laboratory. Prof. Heinz received a B.S. in Physics from Stanford University and a Ph.D. in Physics from the University of California at Berkeley. Subsequently, he was at the IBM Research Division in Yorktown Heights, NY until he joined Columbia University in 1995 as a Professor of Electrical Engineering and Physics. He has also served as a Scientific Director of the Columbia Nanoscale Science and Engineering Center (NSEC) and of the Energy Frontier Research Center (EFRC) until he joined Stanford University in 2015. Prof. Heinz's research focuses on the optical and electronic properties of nanoscale materials, including atomically thin 2D materials such as graphene and ultrathin transition metal dichalcogenide crystals. Using optical and laser spectroscopic techniques, complemented by other physical probes, his lab examines the states of electrons in these systems and learns how they interact with one another, with lattice vibrations, and with other nearby materials. Prof. Heinz is the recipient of APS's Frank Isakson Prize and the Julius Springer Prize for Applied Physics, among other honors.



- PROF. TIMOTHY P. LODGE -

University of Minnesota

#### Monday, September 23, 2019 | 10:30am

La Fonda on the Plaza Ballroom South

#### **Bicontinuous Structures in Charged Polymer Materials**

Nanostructured materials with co-continuous structures, in which each discrete domain is independently interconnected, can simultaneously achieve orthogonal properties such as high molecule or ion transport, and excellent mechanical strength. Potential applications include porous membranes, fuel cells, and rechargeable metal batteries. Block polymers have been exploited as templating agents to access such morphologies, for example via ordered periodic phases such as the double gyroid, or by polymerization-induced microphase separation. In such cases the conducting domains are typically  $\leq$  20 nm in size, and transport can be significantly influenced by the interfacial brush structure. An alternate route involves blending an A-B diblock copolymer with the constituent A and B homopolymers, leading to a disordered bicontinuous microemulsion (B E) state. We have shown that charge-free ternary A-B/A/B polymer blends universally self-assemble into the thermodynamically stable B E phase, albeit with carefully designed molecular weights and compositions. The B E displays globally disordered but locally correlated domains, with tunable characteristic length scales in the range of ca. 20-100 nm, well beyond the domain sizes typically associated with pure diblocks. The interesting question that arises is whether this phase can also be accessed in blends containing charge, where in general the intermolecular interactions are stronger and more long-ranged. We are exploring this issue in two cases: an A-B/A/B ternary system with added salt, and an A-B/A/B system in which one of the polymers is ionomeric.



**Prof. Timothy Lodge** is Regents Professor of Chemistry and Chemical Engineering & Materials Science at the University of Minnesota. Prof. Lodge received a B.A. in Applied Mathematics from Harvard University and Ph.D. in Chemistry from the University of Wisconsin. His research pursues a molecular-level understanding of polymer structure and dynamics. Currently, his lab focuses on multicomponent systems – copolymers, homopolymer blends, and their mixtures – in solution and in the bulk state. The overall scientific challenge is to understand how the thermodynamic interactions among the components control both structure and dynamics. Prof. Lodge is the recipient numerous awards and honors, including: the Paul J. Flory Polymer Education Award from the ACS Division of Polymer Chemistry, honored for his outstanding achievements in promoting undergraduate and graduate polymer education; elected member of the American Academy of Arts and Sciences [AAAS]; and recipient of the Herman F. Mark Polymer Chemistry Award winner for outstanding research in polymer science.



- PROF. RAJIV KALIA -

University of Southern California

#### Monday, September 23, 2019 | 11:10am

La Fonda on the Plaza Ballroom South

#### **Deep Learning in Nanoscience**

Unsupervised learning approaches can greatly benefit synthesis, characterization, modeling and simulation of nanosystems. In this presentation, I will first describe the application of Restricted Boltzmann Machine (RBM) and Variational Autoencoder (VAE) to synthesis and characterization of two-dimensional (2D) layered materials. The RBM is implemented on a quantum annealer, and can correctly identify different phases and defects in the computational synthesis of a MoS2 monolayer by chemical vapor deposition (CVD). The VAE identifies pathways connecting the semiconducting (2H) and metallic (1T) phases via novel intermediate structures called and in a 2D MoWSe2 alloy. These structures are akin to those observed by scanning transmission electron microscopy in a 2D MoS2. The latent-space structures in VAE are combined to form MoWSe2 devices with and interfaces. Quantum simulations show that interfaces synthesized from the latent space in VAE are stable and the devices with those interfaces are suitable for novel nanoelectronics applications. Next, I'll discuss the Weighted Constraint Satisfaction Problem (WCSP) for learning, representation and reasoning across different levels of abstraction in nanosystems. I will demonstrate the success of WCSP methods on imputation of missing data in (a) CVD images of monolayer MoS2, and (b) electron microscopy images. I will also show WCSP results on identifying corrupted parts of electron microscopy images. Lastly, I'll present a novel, extrapolative neural

network called Equation Learner (EQL) for mathematical modeling of experimental and simulation data.



Prof. Rajiv Kalia is Professor of Computer Science, Chemical Engineering, and Materials Science in the USC Viterbi School of Engineering, and Professor of Physics and Astronomy in the USC Dornsife College of Letters, Arts, and Sciences. His multidisciplinary research concentrates in the areas of biophysics and materials science. Prof. Kalia and his team investigate key biophysical processes and related applications for developing new paths in future drug delivery and gene therapies. This work necessitates creating multi-scale simulations of novel materials and biomedical systems through a combination of density functional, molecular dynamics, and finite element computational schemes. Using HPC resources, Kalia has carried out the largest ever all-atom molecular dynamics simulations-on the order of 10 million atoms-that are capable of visualizing water nanobubbles undergoing shockwave-induced collapse and resulting velocity streamlines formed by the subsequent water nanojets. Prof. Kalia is a Fellow of the American Physical Society and has been awarded a Foundation for Fundamental Research on Matter (FOM) Fellowship in the Netherlands; a Sustained Excellence Award in Ultra Dense, Ultra Fast Computing Components from the Defense Advanced Research Projects Agency (DARPA); and a USC Viterbi School of Engineering Senior Research Award. He received his Ph.D. in Physics from Northwestern University in 1976.



- PROF. CHAD A. MIRKIN -

Northwestern University

#### Tuesday, September 24, 2019 | 8:30am

La Fonda on the Plaza Ballroom South

#### Expanding and Exploring the Materials Genome through Cantilever-Free Probe Lithography

Throughout history, the materials we have used and rely on have evolved over time, slowly becoming more and more complex. The progression from the stone tools used by early-man to the polyelemental materials used today has been relatively slow due to the massive parameter space that materials encompass. Indeed, when one considers the 91 metal elements in the periodic table, and all possible combinations, a nearly infinite number of possible materials exist. This is particularly true at the nanoscale where small changes in size or shape, even at a fixed composition, can dramatically change a material's properties. Therefore, the ability to rapidly synthesize and subsequently screen materials for desired properties is needed. In this presentation, a cantilever-free scanning probe lithography approach to combinatorial nanoscience relying on "megalibraries" consisting of as many as 5 billion positionally encoded nanoparticles will be described. The libraries can be tailored to encompass a wide variety of alloy and phase-separated nanoparticles that are comprised of as many as 8 different elements. Importantly, one megalibrary contains more new inorganic materials than scientists cumulatively have produced and characterized to date and can be used to identify new materials and catalysts for important chemical transformations. In addition, from these libraries, important insight into how thermodynamic phases form in polyelemental nanoparticles has been obtained, and design rules for engineering heterostructures in a polyelemental nanoparticle have been established. Therefore, this novel approach lays the foundation for creating an inflection point in the pace at which we both explore the breadth and discover the capabilities of the materials genome.



**Prof. Chad Mirkin** is the Director of the International Institute for Nanotechnology and the George B. Rathmann Professor of Chemistry, Professor of Chemical and Biological Engineering, Professor of Biomedical Engineering, Professor of Materials Science & Engineering, and Professor of Medicine at Northwestern University. He is a chemist and world-renowned nanoscience expert, who is known for the discovery and development of spherical nucleic acids (SNAs) and SNA-based biodetection and therapeutic schemes, the invention of Dip-Pen Nanolithography (DPN) and related cantilever-free nanopatterning methodologies, On-Wire Lithography (OWL), Co-Axial Lithography (COAL), and contributions to supramolecular chemistry and nanoparticle synthesis. Prof. Mirkin has been recognized for his accomplishments with over 210 national and international awards, including the SCI Perkin Medal, the Linus Pauling Medal, and the Dickson Prize in Science, among many others. Prof. Mirkin holds a B.S. from Dickinson College and a Ph.D. in Chemistry from the Pennsylvania State University. He was an NSF Postdoctoral Fellow at the MIT prior to becoming a professor at Northwestern University in 1991.



#### **2019 CINT ANNUAL MEETING**

#### CINT USER EXECUTIVE COMMITTEE USER RECOGNITION AWARD 2019

Over the past 13 years, the Center for Integrated Nanotechnologies (CINT) has been fortunate to work with outstanding researchers from around the world. Our users and staff have collaborated on important advances in many areas of nanoscience, pushing the frontier of knowledge in new and exciting directions.

To recognize such work, CINT's User Executive Committee has established the User Recognition Award. This award honors a CINT user who has built their research program and become a leader in their field through their research at CINT.

We are pleased to announce that the innaugural recipient of this award is Prof. Haiyan Wang (Purdue University). Prof. Wang's research on functional nanocomposite thin films is an excellent example of the innovative and productive work that can result from a user facility collaboration.



#### Prof. Haiyan Wang

Purdue University

Haiyan Wang is Basil S. Turner Professor of Engineering at Purdue University's School of Materials Engineering and School of Electrical and Computer Engineering. She is a Fellow of the MRS, APS, AAAS, ACerS, and ASM, and is the recipient of numerous awards including TAMEST's 2015 O'Donnell Award in Engineering and ASM's 2011 Silver Medal Award for Outstanding Materials Scientist in Mid Career, among others.

Prof. Wang's research interests include nanostructured nitride and oxide thin film heterostructures, coated superconductor materials scale-up and architectures, and microstructural characterization. She has been a CINT user since 2007, during which time she has had 14 user projects. Her CINT research generated 32 peer-reviewed publications during the 2016-2018 review period.

Poster session, Monday September 23, La Terraza at La Fonda User Recognition Award poster: *"Metal-ceramic nanocomposite thin film: Towards tunable 3D structures and multifunctionalities"* 

## CINT USER EXECUTIVE COMMITTEE The voice of CINT users



The CINT User Executive Committee (UEC) is an elected body of current and former CINT users. The UEC takes input from the CINT user community and advocates on behalf of these users to the CINT program management team, regarding:

- Operations
- New capabilities
- Strategic planning
- Proposal reviews

Tito Busani

Mexico

University of New

• Quality of the user experience

Our next election will be held in Fall 2019. If you are interested in serving on the committee, please provide your name and contact information on the meeting feedback form. If you would like to nominate a candidate for the committee, please contact the UEC Chair.

For more information, please visit our website: https://cint.lanl.gov/becoming-user/usersassociation.php

#### **Contact Information:**

- Dr. Erika Vreeland, CINT UEC Chair: erika@irdynamics.com
- Heather Brown, CINT User Program Manager: hdbrown@sandia.gov



**Erika Vreeland** IR Dynamics *Chair and Industrial Advisor* 



**Steven Hayden** Aramco Services Company



Plamen Atanassov University of California, Irvine



**Timothy Lambert** Sandia Ntl. Labs Internal Lab Rep



**Don Lucca** Oklahoma State University *Chair* 



Siddhartha (Sid) Pathak University of Nevada, Reno



**Shalini Tripathi** University of Connecticut *Postdoc Rep* 



Alan Van Orden Colorado State University



#### 2019 CINT ANNUAL MEETING USER EXECUTIVE COMMITTEE SPONSORED WORKING LUNCH

#### - DR. RYAN WIXOM -

Center for Integrated Nanotechnologies

#### Monday, September 23, 2019 | 12:00pm

La Fonda on the Plaza Ballroom South Please collect your lunch from Ballroom North

#### Presentation Zen: Let's free ourselves from bad PowerPoint

As scientists, we spend a significant amount of time watching presentations. Unfortunately, most of the presentations we attend are terrible. If you don't agree, don't worry, I'll tell you why. The good news is that they don't have to be a waste of time. Presentations can actually be an engaging and effective means of communicating our ideas to the scientific community. We just have to change the way we think about presenting our work. I'm going to talk about strategies you can employ to make your presentations engaging, unforgettable, and stimulate meaningful interaction with your audience.



**Dr. Ryan Wixom** is manager of the Nanostructure Physics Department at the Center for Integrated Nanotechnologies (CINT). He received a Ph.D. in Materials Science from the University of Utah, where he studied the use of surfactants to control dopant incorporation during epitaxial growth of III-V semiconductors. After graduating, he joined Sandia as a postdoctoral researcher using density functional theory to study defects in semiconductors. He was subsequently hired into Sandia's Explosives Technology Group, and shifted focus toward the characterization, modeling, and testing of explosive materials. He has an extensive background in modeling, simulation, and characterization of explosives and has developed novel techniques for: microstructural characterization, predicting equations of state, mesoscale hydrodynamic modeling, and utilizing photonic Doppler velocimetry as a diagnostic for small scale shock physics experiments. He is passionate about materials science and applying it's fundamentals to solve multidisciplinary problems. Ryan is active in the international energetic materials community, the Materials Research Society (MRS), and the American Physical Society (APS). He served as the Chair of the 2019 APS Shock Compression of Condensed Matter (SCCM) conference in Portland, OR.



The 2019 CINT Annual Meeting is sponsored, in part, by:

#### Thermo Fisher SCIENTIFIC

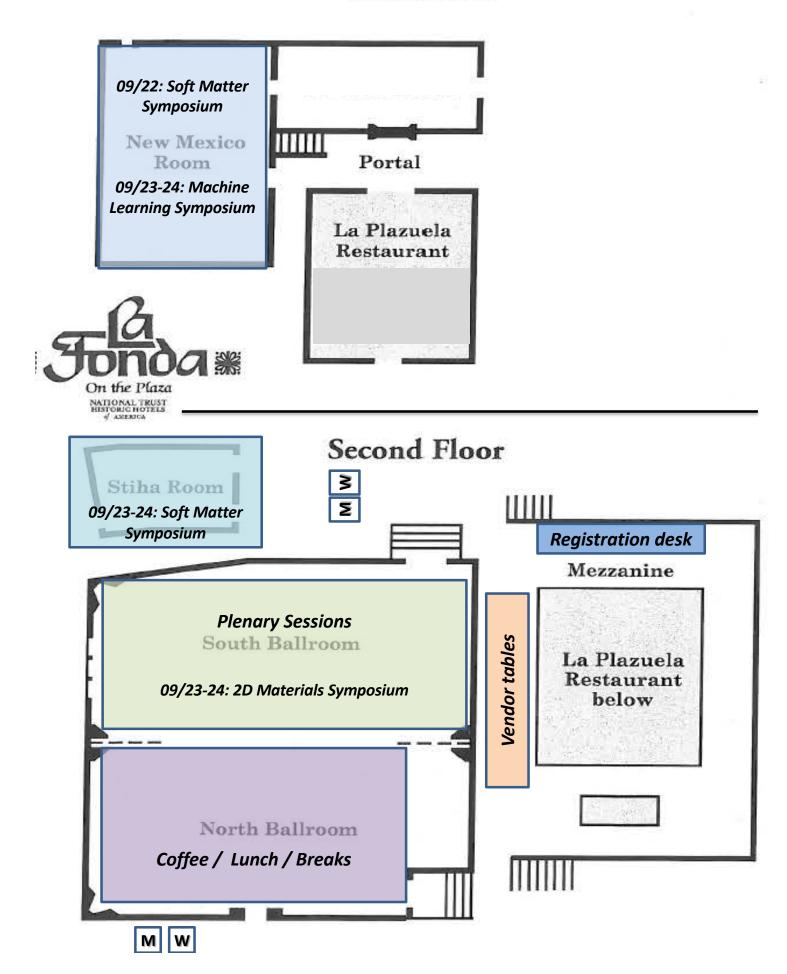


Smart Insight



Thank you for your support!

#### **First Floor**



**Poster Session & Reception** 



Monday, September 23, 2019 5:15pm – 7:00pm

## Thank you to our sponsors for supporting this event!

The CINT poster session will take place on the 3<sup>rd</sup> floor of the hotel, in the La Terraza banquet room & garden patio. Elevators to the terrace are located on the first and second floors near the garage entrance.

One drink ticket per attendee provided courtesy of our sponsors. Thank you!



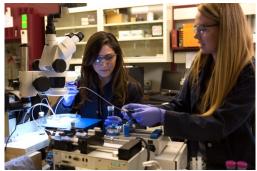


## CINT Call for User Proposals Fall 2019

The Center for Integrated Nanotechnologies (CINT) is a Department of Energy, Office of Science Nanoscale Science Research Center (NSRC) jointly operated by Los Alamos and Sandia national laboratories. As a national user facility, CINT provides approved users access to its staff and capabilities for nanoscale science research at no fee for non-proprietary research. Proprietary research may be conducted under a full-cost recovery agreement.

**Who can be a CINT User** – Individuals and teams from industry, academia, and government institutions are invited to submit proposals to conduct research at CINT. Foreign national users can work at CINT if their visit is planned with sufficient lead-time.

**What is available** – CINT offers world-leading capabilities to create, characterize, and model nanoscale materials in increasingly complex integrated environments. Our comprehensive suite of



capabilities includes the technical expertise, instrumentation and software necessary to address important nanoscience integration problems and obtain high-impact research results. Prospective users should visit the capabilities page on the CINT website (http://cint.lanl.gov/capabilities/index.php) for a brief description of our currently available capabilities. To view a list of capabilities at CINT and all five of the NSRCs, please visit the NSRC portal (https://nsrcportal.sandia.gov/).

**How to apply** – Access to the CINT Core and Gateway Facilities is obtained by submitting a CINT user proposal. These proposals are a concise statement of research that you desire to perform with us at CINT. For more information visit our online step-by-step guide to prepare your CINT user proposal (https://cint.lanl.gov/becoming-user/call-for-proposals.php).

**Proposal Template** – Proposal submissions are required to use our proposal template (https://cint.lanl.gov/becoming-user/call-for-proposals.php). Proposals submitted that do not follow the approved template will not be considered for review. CINT user proposals are evaluated by external reviewers based on <u>six specific proposal elements</u>. All CINT User proposals are expected to explicitly contain the following six elements within the 2-page limit:

1. What are the main scientific questions being addressed in this user project, including the connection to nanoscience? (*Suggested length: 200 words*)

2. Briefly describe the state of research in this area and how your work is advancing the field. (*Suggested length: 150 words*)

3. What is the expected impact of this user project? (Suggested length: 150 words)

4. What specific work will be performed <u>at the user's institution</u> in preparation for, or in support of, the proposed CINT work? (*e.g. sample preparation, complementary characterization, calculations*)

5. What specific tasks will be performed <u>by the user in conjunction with CINT</u>? For each task, include task duration, expected task outcome, requested instrument(s), and CINT staff engagement. (*This should be the longest and most detailed section*.)

6. Key references.

**Proposal Selection** – Proposals will be internally screened for safety/feasibility and prioritized by an external review panel based upon scientific merit and suitability for CINT. Approved proposals will have an 18-month duration. An executed user agreement between CINT and the user institution(s) must be in place prior to starting the approved project. For no-fee access, the project results must be published in peer-reviewed technical publications and include the CINT Acknowledgement statement (available at: http://cint.lanl.gov/publications/index.php).

**Leveraged Capabilities** – In addition to CINT capabilities, prospective users may also request access to a variety of world-class leveraged capabilities hosted at Los Alamos and Sandia National Laboratories. These capabilities include selected ion beam assisted synthesis and characterization techniques, modeling and simulation tools using high performance computing and joint proposals with the National High Field Magnet Laboratory.



**Scientific expertise at CINT** – A distinguishing characteristic of the DOE/SC nanoscience user facilities is the availability of scientific expertise along with hardware/software techniques that enables nanoscience researchers to understand, predict, and realize unprecedented functionalities in materials. CINT expertise is available in these four scientific thrust areas:

- Quantum Materials Systems
- In-situ Characterization and Nano-mechanics
- Nanophotonics and Optical Nanomaterials
- Soft, Biological and Composite Nanomaterials

User proposal submissions: https://cint.sandia.gov/

Submissions accepted: September 1-30, 2019





#### 2019 CINT ANNUAL MEETING - NOTES -









The Center for Integrated Nanotechnologies (CINT) is an Office of Science national user facility jointly operated by Los Alamos and Sandia national laboratories. CINT helps the research community perform cutting-edge research in the area of nanoscience and nanotechnology, with a focus on nanoscience integration. Access to CINT scientists and facilities is available free of charge for open science. As a user facility, CINT has the structure and mission to collaborate widely across industry, academia, and within the DOE labs. Capabilities range from material synthesis and a well-equipped nanofabrication facility, to state-of-the-art imaging, other characterization methods, as well as theory and modelling.