

## ABOUT THE WORKSHOP

This workshop series brings together researchers in electronic structure theory.

Presentations describe new methods for computing previously inaccessible properties, breakthroughs in computational efficiency and accuracy, and novel applications of these approaches to the study of molecules, liquids, and solids.

Since 1989, the Electronic Structure Workshop has been hosted by more than a dozen universities and institutions.

This 30th Anniversary, the workshop returns to the University of Illinois at Urbana-Champaign.

### Electronic Structure Workshop Executive Committee

Jerzy Bernholc (NC State)  
Marco Buongiorno-Nardelli (Univ North Texas)  
Roberto Car (Princeton)  
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James Chelikowsky (UT Austin)  
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John Rehr (Univ Washington)  
Cyrus Umrigar (Cornell)  
David Vanderbilt (Rutgers)  
Shiwei Zhang (William and Mary)

### 2019 Local organizers at the University of Illinois at Urbana-Champaign

Lucas Wagner (Physics)  
André Schleife (MatSE)  
David Ceperley (Physics)

## SPONSORS

We are grateful to the sponsors of the 2019 Workshop:



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# 2019 Workshop on Recent Developments in Electronic Structure

UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN

30TH ANNUAL WORKSHOP • MAY 20-22, 2019

**I** ILLINOIS

# 2019 Workshop on Recent Developments in Electronic Structure

Held at the National Center for Supercomputing Applications  
University of Illinois at Urbana-Champaign • May 20–22, 2019

## MONDAY, MAY 20, 2019

*Talks will be held at the National Center for Supercomputing Applications, Auditorium.*

### 8:45 AM

Workshop Check-in/Badge Pick-up (Atrium)

### 9:00 AM

**André Schleife**, Materials Science & Eng, University of Illinois at Urbana-Champaign  
“Welcome to ES19”

### 9:10 AM

**Peter Abbamonte**, Department of Physics, University of Illinois at Urbana-Champaign  
“Concerning issues about the plasmon lifetime in some correlated metals”

### 9:50 AM

**Karin Rabe**, Department of Physics and Astronomy, Rutgers, The State University of New Jersey  
“Competing phases and functional properties from first principles”

### 10:30 AM

Break

### 11:00 AM

**Noa Marom**, Department of Materials Science and Engineering, Carnegie Mellon University

### 11:40 AM

**Bartomeu Monserrat Sanchez**, Cavendish Laboratory, University of Cambridge  
“The effects of temperature on topological materials”

### 12:20 PM

**Lunch Break on your own**

### 1:50 PM

**Carlo Pierleoni**, Physical and Chemical Sciences, University of L'Aquila  
“Liquid-liquid phase transition in high pressure hydrogen by Quantum Monte Carlo methods”

### 2:30 PM

**Luke Shulenburger**, Sandia National Laboratories  
“Progress from the Methods Development Effort of the Center for the Predictive Simulation of Functional Materials”

### 3:10 PM

Break

### 3:40 PM

**Elif Ertekin**, Mechanical Science and Eng, University of Illinois at Urbana-Champaign  
“First-principles modeling of defects and disorder in materials: some developments and some challenges”

### 4:20 PM

**Linfeng Zhang**, Program in Applied and Computational Mathematics, Princeton University  
“Boosting Ab-initio Molecular Dynamics with Deep Learning”

### 5:00 PM

**Richard Martin**, Department of Physics, Emeritus, University of Illinois; Department of Applied Physics, Stanford University  
“ASESMA: The second decade 2020-2030—New possibilities and opportunities”

### 5:40 PM

**Tutorial on Real Space Multigrid (RMG) version 3.2.** Jerry Bernholc, Emil Briggs and Wenchang Lu, North Carolina State University  
Tutorial group will meet in Atrium after the talks, and walk together to 276 Loomis Lab. Tutorial is free of charge; dinner will be provided.

## TUESDAY, MAY 21, 2019

### 8:45 AM

Workshop Check-in/Badge Pick-up (Atrium)

### 9:00 AM

**Giulia Galli**, Department of Chemistry, The University of Chicago & ANL  
“Coupling first principles molecular dynamics and many body perturbation theory calculations”

### 9:40 AM

**Socrates T. Pantelides**, Department of Electrical Engineering, Vanderbilt University  
“Formation energies of charged defects—resolution of long-standing difficulties”

### 10:20 AM

Break

### 10:50 AM

**Lucas Wagner**, Department of Physics, University of Illinois at Urbana-Champaign  
“Benchmarking high accuracy methods on realistic systems”

### 11:30 AM

**Federico Grasselli**, Scuola Internazionale Superiore di Studi Avanzati  
“Topological quantization and gauge-invariance of charge transport in liquid insulators”

### 12:10 PM

#### Poster Sessions & Lunch

“Meet the Editor” concurrently with posters. No sign-up necessary. Yan Li, Associate Editor, American Physical Society

### 3:10 PM

**Aurora Pribram-Jones**, Chemistry and Chemical Biology, University of California, Merced  
“New Approaches to Temperature-Dependent Density Functional Approximations”

### 3:50 PM

**Joshua Kas**, Department of Physics, University of Washington  
“Finite temperature cumulant Green’s function approach for exchange, correlation, and thermodynamic properties of electronic systems”

### 4:30 PM

**Garnet Chan**, Division of Chemistry and Chemical Engineering, Caltech

### 6:30 PM

**Banquet for registered attendees**  
Location: University of Illinois Alice Campbell Alumni Center, 601 S. Lincoln Avenue, Urbana, IL 61801

## WEDNESDAY, MAY 22, 2019

### 8:45 AM

Workshop Check-in/Badge Pick-up (Atrium)

### 9:00 AM

**William Gropp**, National Center for Supercomputing Applications  
“Challenges in Programming The Next Generation of HPC Systems”

### 9:40 AM

**Vidya Madhavan**, Department of Physics, University of Illinois at Urbana-Champaign  
“Interaction effects and band structure information from quasiparticle interference and Landau level spectroscopy”

### 10:20 AM

Break

### 10:50 AM

**Ye Luo**, Computational Science Division and Argonne Leadership Computing facility, Argonne National Laboratory  
“Getting ready to model material properties at exascale with QMCPACK”

### 11:30 AM

**Yuki Sakai**, Institute for Computational Engineering and Sciences, University of Texas  
“Superconductivity and magnetism in amorphous carbon”

### 12:20 PM

Workshop ends

Visit the website for abstracts and talk slides, when available.  
<http://bit.ly/esw2019>