

*Conference on  
Computational Physics*

CCP2011

OCTOBER 30 - NOVEMBER 3, 2011, GATLINBURG, TENNESSEE

# CONFERENCE ON COMPUTATIONAL PHYSICS 2011

October 30 - November 3, 2011

The Park Vista Hotel  
Gatlinburg, TN, USA

<http://ccp2011.ornl.gov>



INTERNATIONAL UNION OF  
PURE AND APPLIED PHYSICS



CRAY  
THE SUPERCOMPUTER COMPANY



**Scientific Program**

TIME	Sunday 30 Oct	Monday 31 Oct	Tuesday 1 Nov	Wednesday 2 Nov	Thursday 3 Nov
8:00a		<b>REGISTRATION</b> Lower Lobby	<b>REGISTRATION</b> Lower Lobby	<b>REGISTRATION</b> Lower Lobby	<b>REGISTRATION</b> Lower Lobby
8:00a		<b>WORKING CONTINENTAL BREAKFAST</b> Lower Lobby	<b>WORKING CONTINENTAL BREAKFAST</b> Lower Lobby	<b>WORKING CONTINENTAL BREAKFAST</b> Lower Lobby	<b>WORKING CONTINENTAL BREAKFAST</b> Lower Lobby
8:30a		<b>OPENING CEREMONIES</b> STOCKS, MALCOLM HANSEN, ALEX	<b>PLENARY-III</b> SMITH, JEREMY	<b>PLENARY-VII</b> MARTIN, RICHARD	<b>PLENARY-VIII</b> SZALAY, ALEX
9:15a		<b>PLENARY-I</b> GROSS, E.K.U. (HARDY)	<b>PLENARY-IV</b> ORGINOS, KOSTAS	<b>SESSIONS</b> 1.4.3-Tennessee Ballrooms 3&4 2.3-Gardenview A&B 4.1-Gardenview C&D 10.3-Mountainview B 11.1-Mountainview C&D	<b>PLENARY-IX</b> CEPERLEY, DAVID
10:00a		<b>COFFEE BREAK</b> Lower Lobby	<b>COFFEE BREAK</b> Lower Lobby	<b>COFFEE BREAK</b> Lower Lobby	<b>COFFEE BREAK</b> Lower Lobby
10:30a		<b>PLENARY-II</b> DONGARRA, JACK	<b>PLENARY-V</b> SCALETAR, RICHARD	<b>SESSIONS</b> 1.2.1-Tennessee Ballrooms 3&4 1.3.5-Mountainview B 2.4-Gardenview A&B 6.1-Mountainview C&D 7.0-Gardenview C&D	<b>SESSIONS</b> 1.1.2-Mountainview C&D 1.1.3-Gardenview A&B 5.1-Gardenview C&D 8.1-Mountainview B 12.3-Tennessee Ballrooms 3&4
11:15a		<b>SESSIONS</b> 1.3.1-Gardenview A&B 1.6.1-Mountainview C&D 1.7.1-Gardenview C&D 12.1-Tennessee Ballrooms 3&4 10.0-Mountainview B	<b>SESSIONS</b> 1.3.3-Gardenview A&B 1.4.1--Gardenview C&D 1.5.1-Tennessee Ballrooms 3&4 2.1-Mountainview B 10.2-Mountainview C&D		
12:45p		<b>WORKING LUNCH</b> Tennessee Ballrms 1&2 BUCHANAN, MICHELLE ORNL	<b>WORKING LUNCH</b> Tennessee Ballrms 1&2 HANSEN, ALEX Trondheim	<b>WORKING LUNCH</b> Tennessee Ballrms 1&2 STOCKS, MALCOLM ORNL	<b>WORKING LUNCH</b> Tennessee Ballrms 1&2 HANSEN, ALEX Trondheim
2:15p		<b>IUPAP YOUNG SCIENTIST AWARD</b> to CURTAROLO, STEFANO presented by HANSEN, ALEX	<b>PLENARY-VI</b> CARLSON, JOSEPH	<b>TOUR</b> (Optional)	<b>PLENARY-X</b> CHEN, JACQUELINE
3:00		<b>COFFEE BREAK</b> Lower Lobby	<b>COFFEE BREAK</b> Lower Lobby	<b>COFFEE BREAK</b> Lower Lobby	<b>COFFEE BREAK</b> Lower Lobby
3:15p	<b>REGISTRATION</b> Lower Lobby 3:00p-8:00p	<b>SESSIONS</b> 1.1.1-Mountainview C&D 1.7.2-Gardenview C&D 1.3.2-Gardenview A&B 9.1-Tennessee Ballrooms 3&4 10.1-Mountainview B	<b>SESSIONS</b> 1.3.4-Gardenview A&B 1.4.2-Gardenview C&D 2.2-Mountainview B 4.0-Mountainview C&D 12.2-Tennessee Ballrooms 3&4		<b>SESSIONS</b> 1.6.2-Mountainview C&D 7.1-Mountainview B 12.4-Tennessee Ballrooms 3&4 5.2-Gardenview C&D
5:15p					<b>CLOSING CEREMONY</b>
7:45p -			<b>BANQUET</b> Tennessee Ballrooms 1 & 2 MESSER, BRONSON		
8:00a- 11:00a		<b>POSTER SESSION I</b> Tennessee Ballroom 1		<b>POSTER SESSION II</b> Tennessee Ballroom 1	

*Finger foods and drinks will be available at poster sessions*

**SCHEDULE AND SESSION KEY:**

- 1 - Materials/Condensed Matter Theory and Nano Science
  - 1.1.x General
  - 1.2.x Catalysis and Renewable Energy
  - 1.3.x Nuclear Materials
  - 1.4.x Nano Materials
  - 1.5.x Multiscale
  - 1.6.x Conventional and Order N DFT
  - 1.7.x Quantum Monte Carlo
- 2.x - Strongly Correlated Systems and Quantum Phase Transitions
- 3.x - Quantum Chemistry and Atomic Physics
- 4.x - Quantum Chromodynamics
- 5.x - Astrophysics
- 6.x - Plasma Physics
- 7.x - Nuclear and High Energy Physics
- 8.x - Complex Systems – Chaos and Statistical Physics
- 9.x - Macroscopic Transport, Mesoscopic Methods and Related
- 10.x - Biological Physics and Soft Materials
- 11.x - Supercomputing and Computational Physics Teaching
- 12.x - Computational Physics and Sustainable energy

- Plenary Talks: 45 MIN
- Invited Talks: 30 MIN (25 for presentation, 5 for questions)
- Contributed Talks: 20 MIN (15 for presentation, 5 for questions)

# CCP 2011 PROGRAM: CONTENTS

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## Supporting Organizations

International Union of Pure and Applied Physics (IUPAP)  
IUPAP- Commission on Computational Physics (C20)  
American Physical Society - Division of Computational Physics (APS-DCOMP)  
Oak Ridge National Laboratory (ORNL)  
Center for Defect Physics (CDP)  
UT/ORNL Joint Institute for Computational Sciences (JICS)  
Cray Inc.

# HISTORY OF CONFERENCE ON COMPUTATIONAL PHYSICS

CCP 2011– Conference on Computational Physics – to be held in Gatlinburg is the 23rd in an international series of conferences which have served as a lively forum for computational physicists from around the world. Since 1998, the CCP conferences have rotated between the European/African continents, the Asian/Oceanian continents and the Americas.

The CCP series is held jointly under the auspices of the Commission on Computational Physics (C20) of the International Union of Pure and Applied Physics (IUPAP), the Computational Physics Group of the European Physical Society (EPS), and the Division of Computational Physics of the American Physical Society (APS).

In 1997, the CCP conference series succeeded the EPS-APS Joint Conferences "Physics Computing" (PC) organized annually since 1989. This and preceding conferences were:

2011 – Gatlinburg, Tennessee, USA  
2010 – Trondheim, Norway  
2009 - Kaohsiung, Taiwan  
2008 - Ouro Preto, Brazil  
2007 - Brussels, Belgium  
2006 - Gyeongju, Republic of Korea  
2005 - Los Angeles, California, USA  
2004 - Genoa, Italy  
2003 - Beijing, China  
2002 - San Diego, California, USA  
2001 - Aachen, Germany  
2000 - Brisbane, Australia  
1999 - Atlanta, Georgia, USA  
1998 - Granada, Spain  
1997 - Santa Cruz, USA  
1996 - Cracow, Poland  
1995 – Pittsburgh, USA  
1994 - Lugano, Switzerland  
1993 - Albuquerque, USA  
1992 - Prague, Czechoslovakia  
1991 – San Jose, USA  
1990 - Amsterdam, the Netherlands  
1989 – Boston, USA

Succeeding conferences are scheduled for

2012 - Kobe, Japan  
2013 - Moscow

# WELCOME TO CCP 2011

Increasingly, computational physics stands alongside experiment and theory as an integral part of the modern approach to solving the great scientific challenges of the day – from cosmology and astrophysics, through climate science, to materials physics, and the fundamental structure of matter. Computational physics touches aspect of science and technology ranging from the fundamental structures of matter and the universe to the practicalities of delivering communications technologies and securing a clean and efficient energy future. The annual Conferences on Computational Physics (CCP) are dedicated to presenting an overview of the most recent developments and opportunities in computational physics across a broad range of topical areas and from around the world. The CCP series has been in existence more than 20 years, with the most recent gatherings in Ouro Preto, Brazil in 2008, Taiwan in 2009 and Trondheim, Norway in 2010. This year it is my pleasure to welcome you to CCP 2011 and to Gatlinburg, Tennessee, and to autumn in the picturesque Great Smoky Mountains. In keeping with the CCP tradition, the Gatlinburg conference will feature an impressive list of international speakers that will present the latest developments across broad areas of computational physics.

The conference features plenary lectures that are intended to give a broad perspective of the latest developments in a particular field, a full spectrum of parallel sessions featuring a mixture of invited and contributed presentations, as well as poster sessions. At this writing, the conference has more than 225 registered participants and a program consisting of 10 plenary lectures and more than 200 invited and contributed papers and posters with participants representing a total of 44 nationalities.

On Monday and Wednesday evenings, we will have poster sessions that will feature extensive hors d'oeuvres and bar. The conference banquet on Tuesday evening will provide a further social function along with a dinner talk that should be of interest to participants and guests.

I hope that many of you will take the opportunity to see some of the surrounding area, particularly the Great Smoky Mountain National Park. Hopefully, mother nature will be kind enough to allow some of the fall colors to hang around for your enjoyment.

In closing, let me express my appreciation for you taking time out of your busy schedules to attend CCP 2011. Particular thanks are also due to the committees that have help put the conference together, especially the local organizing committee and a number of ORNL staff who have spend long hours with the administrative details.

Best wishes for an enjoyable conference.

G. Malcolm Stocks  
Oak Ridge National Laboratory  
CCP 2011 Conference Chair

## CONFERENCE ORGANIZATION

**Chair:** Dr. Malcolm Stocks (ORNL)

**Vice Chairs:** Adriana Moreo (ORNL/UT); James Gubernatis (LANL)

**Conference Administrator:** Ann Strange (ORNL)

### Local Program Committee:

Don Batchelor (ORNL)

Jack Dongarra (UTK/ORNL)

James Hack (ORNL)

Robert Harrison (ORNL)

Paul Kent (ORNL)

Anthony Mezzacappa (ORNL)

Adriana Moreo (ORNL)

Witold Nazarewicz (UT)

Loukas Petridis (ORNL)

David Schultz (ORNL)

Bill Shelton (PNNL)

Claudia Troparevsky (UT/ORNL)

Mina Yoon (ORNL)

### International Advisory Board Members

Joan Adler (Israel Inst. Tech.)

Constantia Alexandrou (U. Cyprus)

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Giulia A. Galli (UC Davis)

Gillian Gehring (U. Sheffield)

Guang-Yu Guo (Taiwan U.)

Sharon Hammes-Schiffer (Penn St. U.)

Alex Hansen (NUST)

Duane D. Johnson (UIUC)

David Landau (U. Georgia)

Joaquin Marro (U. Granada)

Richard Martin (UIUC, US)

Todd Martinez (Stanford U.)

Bill McCurdy (LBNL)

Ingrid Mertig (Martin Luther U.)

Alejandro Muramatsu (U. Stuttgart)

Richard Needs (Cavendish Lab.)

Giuseppina Orlandini (U. Trento)

Martin Savage (U. Washington)

Thomas Schulthess (ETH)

Dzidka Szotek (Daresbury Lab.)

Hideaki Takabe (Osaka U.)

William M. Tang (Princeton U.)

James Vary (Iowa St. U.)

Enge Wang (Chinese Acad. Sci.)

Jian-Guo Wang (IAPCM)

Jian-Sheng Wang (National U.)

Dan Wei (Tsinghua U.)

Tony Williams (U. Adelaide)

Rudy Zeller (Julich)

# SOCIAL PROGRAM

## Accompanying Persons

While no specific program has been arranged for accompanying persons in Gatlinburg, the surrounding areas of natural beauty provide ample opportunity for visitor enjoyment. The CCP conference desk, the hotel reception, and the Gatlinburg Visitors Bureau will be available to advise visitors regarding local attractions.

Please contact either the CCP 2011 conference desk or hotel staff for information regarding the **complementary shuttle bus** from the conference hotel to various points of interest in the Gatlinburg environs.

## Conference Banquet and Speaker

The conference banquet will be held on Tuesday evening beginning at 7:45 pm and guests of conference participants are welcome\*. Dr. Bronson Messer from the Oak Ridge Leadership Computing Facility (OLCF) will present the dinner address, "Tales from the Bleeding Edge and why you should care."

\* A fee of \$60 will be charged for each guest.

## Smoky Mountains Bus Tour

Conference participants may enjoy an optional coach tour of Great Smoky Mountains National Park on Wednesday afternoon. A coach will depart from in front of the hotel at 2pm and return in the early evening. Depending on the weather and conditions, the coach will visit Clingman's Dome, the highest road-accessible location in the park, then descend to the mountain farm museum near Cherokee, North Carolina. A warm coat or jacket is recommended for the top of the mountain.

The optional tour costs \$20 and must be paid and registered for by Monday evening at the conference registration desk.

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*(Please fill in information and return to Registration Desk by Monday at 8:00 pm)*

I would like to go on the Bus Tour on Wednesday at 2:00.

Name: \_\_\_\_\_

Organization: \_\_\_\_\_

Number of People: \_\_\_\_\_ Payment: \$ \_\_\_\_\_

*(For Registration Staff Only):* Paid: \$ \_\_\_\_\_ Via: \_\_\_\_\_ Date: \_\_\_\_\_



# INSTRUCTIONS AND GUIDELINES FOR SESSION CHAIRS AND PRESENTERS

## **Session Chairs and Presenters: Oral Sessions**

**Session Chairs:** Please keep the sessions on schedule so that each speaker gets their allotted time. Cut off speakers and QA sessions to ensure that the session remains on schedule. If a speaker is not present, take a break so that the session remains as scheduled.

**Presenters:** If possible please test your computer with the available equipment prior to the session. Please stay within your time allocation (45 minutes for plenary presentations, 30 minutes for invited presentations; 20 minutes for contributed talks) allowing at least five minutes for questions and discussion.

## **Presenters: Poster Sessions**

On the day of your poster session, please post your contribution during the day (the poster boards will remain available from early morning). Please stay at your poster for the full session to encourage participation by all conference attendees. A “Best Poster” ballot will be provided during both poster sessions and the winners announced the next day.

Finger food and bar will be provided. At registration each participant will receive tickets for (two) complementary drinks; additional drinks can be purchased at the cash bar.

## **Authors of Proceedings Papers**

Papers presented at CCP 2011 are eligible for publication in the *Journal of Physics: Conference Series*. *The Journal of Physics: Conference Series* is an open access journal that will provide fast publication of the CCP 2011 Proceedings. In addition to the standard benefits of publication in an IOP journal (reviewed, abstracted and indexed in Web of Science), JPCS allows the submission of supplemental materials including color illustrations, codes and movies that can substantially enhance the value your paper.

Details regarding the submission and review process can be found on the CCP 2011 website. All papers should be submitted directly to the conference organizers using the conference website upload. All papers should be prepared using one of the templates (Microsoft Word, Latex) available from the *Journal of Physics: Conference Series* website. A PDF version of the paper should be used for initial submission. Final documents and supplemental materials should only be submitted following peer review.

**Submission Deadline: December 1st 2011.**

# **Daily**

# **Schedules**

**Opening Ceremonies**  
**Monday 31 October: 8:30 (Tennessee Ballrooms 1&2)**  
**Chairperson: G. Malcolm Stocks and Alex Hansen**

**Plenary I & II**  
**Monday 31 October: 9:15 and 10:30 AM (Tennessee Ballrooms 3&4)**  
**Chairperson: Robert Harrison**

Time	Title	First Name	Last Name	Affiliation
9:15 AM	Physics on the Femto-Second Time Scale: Analysis and Control of Electronic Motion	E.K.U.	Gross	Max Planck Institute, Halle, Germany
10:30 AM	On the Future of High Performance Computing: How to Think for Peta and Exascale Computing	Jack	Dongarra	UT/ORNL, USA

**Oral Session 1.3.1 Nuclear Materials**  
**Monday 31 October: 11:15 AM - 12:45 PM (Gardenview A&B)**  
**Chairperson: Roger Stoller**

Time	Title	First Name	Last Name	Affiliation
11:15 AM (I)	Interatomic Forces. Practical methods beyond EAM	Graeme	Ackland	University of Edinburgh, UK
11:45 AM (I)	Stochastic methods for diffusion-reaction simulations of irradiated materials	Vasily	Bulatov	Lawrence Livermore National Laboratory, USA
12:15 PM (I)	The influence of interface sink strength on the reduction of radiation-induced defect concentrations and fluxes in materials with large interface area per unit volume	Michael	Demkowicz	Massachusetts Institute of Technology, USA

**Oral Session 1.6.1 Conventional and Order N DFT**  
**Monday 31 October: 11:15 AM - 12:45 PM (Mountainview C&D)**  
**Chairperson: Andrew Canning**

Time	Title	First Name	Last Name	Affiliation
11:15 AM (I)	Linear scaling approaches for density functional calculations	Rudolf	Zeller	Institute of Advanced Simulation, Forschungszentrum Jülich GmbH
11:45 AM (I)	Resiliency in massively parallel quantum simulations	Thomas	Schulthess	ETH Zurich, Switzerland
12:15 PM	Spectral element formulation of density functional theory	Kristopher	Andersen	High Performance Technologies, Inc., USA

**Oral Session 1.7.1 Quantum Monte Carlo**  
**Monday 31 October: 11:15 AM - 12:45 PM (Gardenview C&D)**  
**Chairperson: Fernando Reboredo**

Time	Title	First Name	Last Name	Affiliation
11:15 AM (I)	Experiments with the full configuration interaction quantum Monte Carlo method	William Matthe	Foulkes	Imperial College London, UK

(I) Invited talk

11:45 AM (I)	Ab initio simulations in quantum many-body systems by auxiliary fields	Shiwei	Zhang	College of William & Mary, USA
12:15 PM (I)	Quantum Monte Carlo methods: many-body nodal structures and treating the spins	Lubos	Mitas	North Carolina State University, USA

**Oral Session 12.1 Computational Physics and Sustainable Energy**  
**Monday 31 October: 11:15 AM - 12:45 PM (Tennessee Ballrooms 3&4)**  
**Chairperson: Mina Yoon**

Time	Title	First Name	Last Name	Affiliation
11:15 AM (I)	Ferroelectricity in Perovskites	David	Singh	ORNL, Oak Ridge, USA
11:45 AM (I)	First-Principles Studies of Loss Mechanisms in Nitride Light Emitters	Chris	Van de Walle	University of California, Santa Barbara, USA
12:15 PM	Modelling of solar energy storage using chemical heat pumps	Yannick	De Decker	Université Libre de Bruxelles

**Oral Session 10.0 Biological Physics and Soft Materials**  
**Monday 31 October: 11:15 AM - 12:45 PM (Mountainview B)**  
**Chairperson: Loukas Petridis**

Time	Title	First Name	Last Name	Affiliation
11:15 AM (I)	Molecular mechanism of allosteric regulation of an intrinsically disordered protein, sortase, revealed by comprehensive all-atom conformational sampling simulations	Kei	Moritsugu	RIKEN, Japan
11:45 AM	Block copolymer self-assembly: A coarse grain computational approach	Goundla	Srinivas	ORNL, Oak Ridge, USA
12:05 PM	Conformational transitions of a confined lattice protein: A Wang-Landau study	Busara	Pattanasiri	University of Georgia, USA; Mahidol University, Bangkok, Thailand

**Working Lunch**  
**Speaker: Michelle Buchanan, ORNL**  
**"Overview of Computational Physics at ORNL"**

**Presentation of the Young Scientist Award**  
**Monday 31 October: 2:15 PM - 3:00 PM (Tennessee Ballrooms 3&4)**  
**Chairperson: Alex Hansen**

Time	Title	First Name	Last Name	Affiliation
2:15 PM	IUPAP: Thermodynamic and kinetic effects in nano-catalysts	Stefano	Curtarolo	Duke University, USA

**Oral Session 1.1.1 Materials /Condensed Matter Theory and Nano Science: General**  
**Monday 31 October: 3:15 PM - 5:15 PM (Mountainview C&D)**  
**Chairperson: Markus Eisenbach**

Time	Title	First Name	Last Name	Affiliation
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(I) Invited talk

3:15 PM	Simulating metal oxides and their heterointerfaces with screened hybrid density functional theory	Fadwa	El-Mellouhi	Texas A&M University at Qatar
3:35 PM	Ab initio molecular dynamics study of diffusion mechanism in liquid B <sub>2</sub> O <sub>3</sub> under pressure	Satoshi	Ohmura	Kumamoto University, Japan
3:55 PM	Numerical closure for chemically reacting systems with lateral interactions	Giacomo	Mazzi	Scientific Computing, K.U. Leuven, Belgium
4:15 PM	Molecular dynamics simulation of phonon transport in the Green-Kubo formalism of thermal conductivity	Hideo	Kaburaki	Japan Atomic Energy Agency, Japan
4:35 PM	Estimation of Ground Behavior Using Kalman Filter Finite Element Method	Masahide	Nakatani	Chuo University, China
4:55 PM	Enumeration of isopointal sets as subspaces for structural search	Toby	Hudson	The University of Sydney, Australia

**Oral Session 9.1 Macroscopic Transport, Mesoscopic Methods and Related**  
**Monday 31 October: 3:15 PM - 5:15 PM (Tennessee Ballrooms 3&4)**  
**Chairperson: TBD**

Time	Title	First Name	Last Name	Affiliation
3:15 PM (I)	Coupling a Fluctuating Fluid with Suspended Structures	Aleksandar	Donev	New York University, USA
3:45 PM	Dependence of the fluid convection in an evaporating sessile droplet on the thermal conductivity of the substrate	Lev	Barash	Landau Institute for Theoretical Physics, Russia
4:05 PM	HPC Discrete Ordinates Method for the solution of 3D radiative transfer	William F.	Godoy	NASA Langley Research Center, USA
4:25 PM	Semi-Lagrange Galerkin Method for Advection Diffusion Problem	Tomoya	Herai	Chuo University, China
4:45 PM	Statistical Law of Turbulence in Granular Gas	Masaharu	Isobe	Nagoya Institute of Technology, Japan
5:05 PM	An Identification of Geological Boundaries Using First-order Adjoint Equation Method	Shigenori	Mikame	Chuo University, China

**Oral Session 1.7.2 Quantum Monte Carlo**  
**Monday 31 October: 3:15 PM - 5:15 PM (Gardenview C&D)**  
**Chairperson: Matthew Foulkes**

Time	Title	First Name	Last Name	Affiliation
3:15 PM (I)	(Abstract not available)	Sandro	Sorella	SISSA, Italy
3:45 PM (I)	Quantum Monte Carlo calculations of defects in aluminum	Randy	Hood	Lawrence Livermore National Laboratory, USA
4:15 PM	Hybrid algorithms in quantum Monte Carlo	Jeongnim	Kim	University of Illinois at Urbana-Champaign, USA

**Oral Session 1.3.2 Nuclear Materials**  
**Monday 31 October: 3:15 PM - 5:15 PM (Gardenview A&B)**  
**Chairperson: Bill Weber**

(I) Invited talk

Time	Title	First Name	Last Name	Affiliation
3:15 PM (I)	The unreasonable effectiveness of mathematical models for nuclear materials	Sergei	Dudarev	University of Oxford, UK
3:45 PM (I)	Theory of radiation dAMage in solids: From oversimplified to predictive general frAMework	Stanislav	Golubov	ORNL, Oak Ridge, USA
4:15 PM (I)	Some properties of radiation induced defects and their effect to mechanical response of irradiated metals	Yury	Osetskiy	ORNL, Oak Ridge, USA

**Oral Session 10.1 Biological Physics and Soft Materials**  
**Monday 31 October: 3:15 PM - 5:15 PM (Mountainview B)**  
**Chairperson: Loukas Petridis**

Time	Title	First Name	Last Name	Affiliation
3:15 PM (I)	Crystal nucleation kinetics revealed by the reweighted path ensemble	Peter	Bolhuis	University of Amsterdam, The Netherlands
3:45 PM	Surface adsorption of lattice HP proteins: studies on thermodynamics and structural transitions using Wang-Landau sampling	Ying Wai	Li	Center for Simulational Physics, University of Georgia, USA
4:05 PM	The influence of the anchoring energy strength on the hysteresis of light induced Fredericksz transition in confined light beams	Oleksandr	Tarnavskyy	Taras Shevchenko National University of Kyiv, Ukraine
4:25 PM	Dynamic heterogeneity of temperature dependent dynamics of Cytochrome P450cam	Zheng	Yi	ORNL, Oak Ridge, USA/UT Center for Molecular Biophysics

**Poster Session I**  
**Monday 31 October: 8:00 - 11:00 PM (Tennessee Ballroom 1)**

Session ID	Title	First Name	Last Name	Affiliation
P1.1	Computer Aided Design of Optimized Magnetic Lens in FIB System by mixing DynAMic ProgrAMming and AI techniques	Fadhil	Ali	Basra University, Basra
P1.2	The dynamic three-dimensional models GaAs	Kulpash	Iskakova	Rif Akhmaltdinov, Russia
P1.3	Structural and electronic properties of MgxCd1-xO: A first-principles study	Dr. K.B.	Joshi	M.L. Sukhadia University, Udaipu, India
P1.4	DynAMical behavior of volatilities in futures exchange markets	Kyungsik	Kim	Pukyong National University, Korea
P1.5	Analysis of a seismic network against spatial shifts and scales in volume	Kyungsik	Kim	Pukyong National University, Korea

(I) Invited talk

P1.6	Surface nitrogenation tuning the thermal conductivity of silicon nanowires: a molecular dynamics study	Haipeng	Li	City University of Hong Kong, Hong Kong SAR, People's Republic of China.
P1.7	A Tersoff potential with modified cutoff for pure and hydrogenated AMorphous carbon and the friction laws at the nanoscale	Zhendong	Sha	Institute of High Performance Computing, Singapore
P1.8	Wave Packet Molecular DynAMics with Packet Splitting	Ilya	Valuev	Joint Institute for High Temperatures of RAS, Russia
P1.9	Towards ab initio simulation of large materials sAMples at 10 nm scale	Yang	Wang	Pittsburgh Supercomputing Center, USA
P1.10	Identification of full order parAMeter and conjugate field in the dynamic phase transition in the mean-field Ginzburg-Landau model	Daniel	Robb	Berry College, Georgia, USA
P1.11	Cluster Bundlet Model of Single-Wall C, BC_2N and BN Nanotubes, Nanocones and Nanohorns	Francisco	Torrens	Universitat de Valencia-ICMol, Spain
P1.12	Ab-initio determination of X-ray structure factors of fcc-copper	Parvej	Alvi	Department of Physics, Banasthali University, India
P1.13	GRMHD simulations of binary neutron-star mergers	Luca	Baiotti	Institute of Laser Engineering, Osaka University, Japan
P1.14	Pseudorandom number generators for Monte Carlo simulations: equidistribution property, statistical independence of bits and effective implementations using SIMD parallelism of modern CPUs	Lev	Barash	Landau Institute for Theoretical Physics, Chernogolovka, Russia
P1.15	Finding Vacancies in a Defected Crystal	George	Bargoud	Pittsburgh Supercomputing Center, USA
P1.16	Simulation of surface dAMage from ion irradiation	GrahAM	Galloway	Edinburgh University, UK
P1.17	"Conveyor Belt" Model for Interfacial Cracks	Knut	Gjerden	Norwegian University of Science and Technology
P1.18	Local strain effect on graphene by a first-principles study	Gui	Gui	University of Wisconsin-Madison, USA
P1.19	Electronic properties of rippled graphene	Gui	Gui	University of Wisconsin-Madison, USA
P1.20	Computer simulation of fluorescence spectra for molecular ring: Localization of exciton states	Pavel	Herman	Faculty of Science, University of Hradec Kralove, Czech Republic

(I) Invited talk

P1.21	How does water boost the protein internal motion	Liang	Hong	Center of Molecular Biology, ORNL, Oak Ridge, USA
P1.22	QMC calculations on ThO molecule and ThO <sub>2</sub> crystal	Shuming	Hu	North Carolina State University, USA
P1.23	Symbolic programming package \textit{NCoperators} with applications in atomic physics	Rytis	Jursenas	Institute of Theoretical Physics and Astronomy of Vilnius University, Vilnius, Lithuania
P1.24	Grain-Boundary Diffusion and Segregation of Hydrogen in Iron: A Path-Integral Molecular DynAMics Study	Hajime	Kimizuka	Department of Mechanical Science and Bioengineering, Osaka University, Japan
P1.25	Modeling Charged Systems in Periodic Boundary Conditions	Jaron	Kroegel	University of Illinois at Urbana-Champaign, USA
P1.26	Extending the length scales of many-body simulations with density-functional calculations	Fengjie	Ma	College of William and Mary, USA
P1.27	The Reprocessing Plant Toolkit: A Unified Framework for Modeling and Simulation of Spent Nuclear Fuel Reprocessing	Alexander	McCaskey	ORNL, Oak Ridge, USA
P1.28	Validity of the scattering length approximation in strongly interacting Fermi systems	ShengQuan	Zhou	University of Illinois at Urbana-Champaign, USA
P1.29	Energy Relaxation Behavior of Optically Generated Hot Carriers in GaN	Kyung Soo	Yi	The Univ. of Texas at Dallas; Pusan National University, Korea

**Plenary III, IV and V**  
**Tuesday 1 November: 8:30, 9:15, and 10:30 (Tennessee Ballrooms 3&4)**  
**Chairperson: Loukas Petridis, Martin Savage, Thomas Maier**

Time	Title	First Name	Last Name	Affiliation
8:30 AM	Computational Physics of Biomolecules	Jeremy	Smith	ORNL, Oak Ridge, USA
9:15 AM	Hadronic Physics from Lattice QCD	Kostas	Orginos	College of William & Mary, USA
10:30 AM	Quantum Monte Carlo in Condensed Matter Physics: Past, Present, and Future	Richard	Scalettar	Univ. of California, Davis, USA

**Oral Session 1.3.3 Nuclear Materials**  
**Tuesday 1 November: 11:15 am - 12:45 pm (Gardenview A&B)**  
**Chairperson: Graeme Ackland**

Time	Title	First Name	Last Name	Affiliation
11:15 AM (I)	Multiscale Modeling Framework in Simulating Radiation Damage	Roger	Stoller	ORNL, Oak Ridge, USA
11:45 AM (I)	Charge Transfer and Redistribution during Low-Energy Recoil Events	William	Weber	University of Tennessee, USA
12:15 PM (I)	Applications of the dislocation dynamics method to irradiation hardening in metals	Jaime	Marian	Lawrence Livermore National Laboratory, USA

**Oral Session 1.4.1 Nano Materials**  
**Tuesday, 1 November: 11:15 am - 12:45 pm (Gardenview C&D)**  
**Chairperson: Cecilia Noguez**

Time	Title	First Name	Last Name	Affiliation
11:15 AM (I)	Approaches for the simulation of open quantum systems and quantum computation with time-dependent density functional theory	Alan	Aspuru-Guzik	Harvard University, USA
11:45 AM	Surface plasmonics in surfaces patterned/structured by nanoparticles	Paul Anton	Letnes	Norwegian University of Science and Technology
12:05 PM	Atomistic simulations of vibration of carbon nanotubes: is it possible to measure the mass of single atom?	Polina	Pine	Russell Berrie Nanotechnology Institute, Technion

**Oral Session 1.5.1 Multiscale**  
**Tuesday 1 November: 11:15 am - 12:45 pm (Tennessee Ballrooms 3&4)**  
**Chairperson: Thomas Schulthess**

Time	Title	First Name	Last Name	Affiliation
11:15 AM (I)	Interatomic potentials and quantum mechanical models	Gabor	Csanyi	Cambridge University, UK
11:45 AM (I)	Adsorption of polyvinylpyrrolidone on Ag surfaces: Insight into the workings of a structure-directing agent	Kristen	Fichthorn	Penn State University, USA
12:15 PM (I)	Fully ab initio determination of free energies: Methodological challenges and applications	Jorg	Neugebauer	Max-Planck-Institut für Eisenforschung GmbH

(I) Invited talk

**Oral Session 2.1 Strongly Correlated Systems and Quantum Phase Transitions****Tuesday 1 November: 11:15 am - 12:45 pm (Mountainview B)****Chairperson: Zlatko Papic**

Time	Title	First Name	Last Name	Affiliation
11:15 AM (I)	Real Space Entanglement Spectrum of Fractionally Quantized Hall States	Edward	Rezayi	California State University, Los Angeles, USA
11:45 AM (I)	Bi-partite composite fermion model for the 5/2 fractional quantum Hall state	Arkadiusz	Wosj	Wroclaw University, Poland
12:15 PM	Universality of Edge Physics in the Fractional Quantum Hall Regime: Contrasting Graphene with Gallium Arsenide	Zixiang	Hu	Princeton University, USA

**Oral Session 10.2 Biological Physics and Soft Materials****Tuesday 1 November: 11:15 am - 12:45 pm (Mountainview C&D)****Chairperson: Jeremy Smith**

Time	Title	First Name	Last Name	Affiliation
11:15 AM (I)	Insights from biophysical studies of intrinsically disordered proteins	Rohit V.	Pappu	Washington Univ., Missouri, USA
11:45 AM (I)	Integrative Modeling of Protein/DNA Complexes at the Replication Fork	Ivaylo	Ivanov	Georgia State University, USA
12:15 PM	Modulation of the Dynamics of Proteins and Related Functions via pH Changes	Sunita	Negi	Sabanci University, Istanbul, Turkey

**Working Lunch****Speaker: Alex Hansen, Norwegian University of Science and Technology  
"IUPAP and C20"****Plenary VI****Tuesday 1 November: 2:15 pm (Tennessee Ballrooms 3&4)****Chairperson: Witold Nazarewicz**

2:15 PM	Recent Advances in Quantum Monte Carlo for Nuclei and Cold Atoms	Joseph	Carlson	Los Alamos National Laboratory, USA
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**Oral Session 1.3.4 Nuclear Materials****Tuesday, 1 November: 3:15 pm - 5:15pm (Gardenview A&B)****Chairperson: Blas Uberuaga**

Time	Title	First Name	Last Name	Affiliation
3:15 PM (I)	Fundamental Materials Science Challenges for Next-Generation Nuclear Energy Systems	Steve	Zinkle	ORNL, Oak Ridge, USA
3:45 PM (I)	Quantum mechanical simulations of electronic stopping in metals	Daniel	Mason	Imperial College London, UK

**Oral Session 1.4.2 Nano Materials****Tuesday 1 November: 3:15 pm - 5:15pm (Gardenview C&D)****Chairperson: Juan C. Idrobo**

Time	Title	First Name	Last Name	Affiliation
3:15 PM (I)	Tuning Transport Properties of Graphene Systems	Jianxin	Zhong	Xiangtan University, China

(I) Invited talk

3:45 PM	I-V Characteristics of Doped Carbon Nanotubes	Shoichi	Sakamoto	Seikei University, Japan
4:05 PM	Electron Transfer on Impurity doped Graphene Nanoribbon	Hiroyoshi	Tsuyuki	Seikei University, Japan
4:25 PM	Nanofluidics in Carbon Nanotubes	Titus	Beu	University Babes-Bolyai, Cluj-Napoca, Romania

**Oral Session 2.2 Strongly Correlated Systems and Quantum Phase Transitions**  
**Tuesday 1 November: 3:15 pm - 5:15 pm (Mountainview B)**  
**Chairperson: Edward Rezayi**

Time	Title	First Name	Last Name	Affiliation
3:15 PM (I)	Numerical studies of the fractional quantum Hall effect in two-dimensional chiral electron systems	Zlatko	Papic	Department of Electrical Engineering, Princeton University
3:45 PM (I)	Non-Abelian anyons and the fractional quantum Hall effect at filling $5/2$	Michael	Peterson	California State University Long Beach
4:15PM (I)	From fractional quantum Hall to fractional Chern Insulators	Nicolas	Regnault	CNRS, Paris, France

**Oral Session 4.0 Quantum Chromodynamics**  
**Tuesday 1 November: 3:15 pm - 5:15 pm (Mountainview C&D)**  
**Chairperson: Charles Horowitz**

Time	Title	First Name	Last Name	Affiliation
3:15 PM (I)	(Abstract not available)	Martin	Savage	University of Washington, USA
3:45 PM (I)	The Spectrum of QCD using lattice gauge theory	David	Richards	Jefferson Lab, USA
4:15 PM (I)	Nuclear Physics from lattice QCD	Robert	Edwards	Jefferson Lab, USA
4:45 PM (I)	Challenges and Opportunities for Lattice QCD software	Balint	Joo	Jefferson Lab, USA
5:15 PM	The Search for New Physics with Lattice Gauge Theory	Paul	Mackenzie	Fermilab, USA

**Oral Session 12.2 Computational Physics and Sustainable Energy**  
**Tuesday 1 November: 3:15 pm - 5:15pm (Tennessee Ballrooms 3&4)**  
**Chairperson: Nicola Marzari**

Time	Title	First Name	Last Name	Affiliation
3:15 PM (I)	New Materials for Solar Thermal Capture and Storage	Jeffery	Grossman	Massachusetts Institute of Technology, USA
3:45 PM (I)	Harvesting solar energy: DFT studies of organic photovoltaics and photo-catalytic water splitting	Harald	Oberhofer	Technical University, Munich, Germany
4:15 PM (I)	Challenges for density-functional theory in modelling materials for energy applications	Nicola	Marzari	University of Oxford, UK
4:45 PM (I)	Graphene systems under external perturbations	Young-Woo	Son	KIAS, Seoul, Korea

(I) Invited talk

**Banquet**

**Tuesday 1 November: 7:00 - 9:00 pm (Tennessee Ballrooms 1&2)**

**Speaker: Bronson Messer**

**Plenary VII**  
**Wednesday 2 November: 8:30 am (Tennessee Ballrooms 3&4)**  
**Chairperson: Joan Adler**

Time	Title	First Name	Last Name	Affiliation
8:30 AM	African School on Electronic Structure Methods and Applications (ASESMA)	Richard	Martin	University of Illinois and Stanford University, USA

**Oral Session 1.4.3 Nano Materials**  
**Wednesday 2 November: 9:15 am - 10:15 am (Tennessee Ballrooms 3&4)**  
**Chairperson: De-en Jiang**

Time	Title	First Name	Last Name	Affiliation
9:15 AM (I)	Modelling of Role of Kinetics and Thermodynamics in Determining the Nanomorphology of Gold	Amanda	Barnard	CSIRO Materials Science & Engineering, Australia
9:45 AM	Energy Landscape of Fullerene Materials: A Comparison of Boron to Boron Nitride and Carbon	Sandip	De	Universität Basel, Basel, Switzerland

**Oral Session 2.3 Strongly Correlated Systems and Quantum Phase Transitions**  
**Wednesday 2 November: 9:15 am - 10:15 am (Gardenview A&B)**  
**Chairperson: Adriana Moreo**

Time	Title	First Name	Last Name	Affiliation
9:15 AM (I)	Material specific Hamiltonian approach to iron-based and cuprate high Tc superconductors	Kazuhiko	Kuroki	The University of Electro-Communications, Japan
9:45 AM (I)	Progress in the computational search for higher-Tc superconductors	Thomas	Maier	ORNL, Oak Ridge, USA

**Oral Session 4.1 Quantum Chromodynamics**  
**Wednesday 2 November: 9:15 am - 10:15 am (Gardenview C&D)**  
**Chairperson: TBD**

Time	Title	First Name	Last Name	Affiliation
9:15 AM (I)	Progress in lattice QCD at non-zero temperature and density	Peter	Petreczky	Brookhaven National Lab, USA
9:45 AM (I)	Lattice QCD for Precision Nucleon Matrix Elements	Huey-Wen	Lin	University of Washington, USA

**Oral Session 10.3 Biological Physics and Soft Materials**  
**Wednesday 2 November: 9:15 am - 10:15 am (Mountainview B)**  
**Chairperson: Loukas Petridis**

Time	Title	First Name	Last Name	Affiliation
9:15 AM (I)	Bridging Scales in Biology: From Atoms to Populations	Eugene	Shakhnovich	Harvard University, USA

(I) Invited talk

9:45 AM (I)	Two molecular dynamics applications: (a) simulations of the Pdx1 homeodomain; (b) investigation of the $\alpha$ -sheet secondary structure	Volodymyr	Babin	North Carolina State University, USA
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**Oral Session 11.1 Supercomputing and Computational Physics Teaching**  
**Wednesday 2 November: 9:15 am - 10:15 am (Mountainview C&D)**  
**Chairperson: Richard Martin**

Time	Title	First Name	Last Name	Affiliation
9:15 AM (I)	Webpage preparation as a tool in (Computational) Physics Education	Joan	Adler	Technion - Israel Institute of Technology
9:45 AM	An eTextBook in Computational Physics with Multiple Executable Elements	Rubin H	Landau	Oregon State University, USA

**Oral Session 1.2.1 Catalysis and Renewable Energy**  
**Wednesday 2 November: 10:30 am - 12:45 pm (Tennessee Ballrooms 3&4)**  
**Chairperson: M. Claudia Tropsch**

Time	Title	First Name	Last Name	Affiliation
10:30 AM (I)	First principles simulations of materials and processes in photo- and electro-catalysis	Annabella	Selloni	Princeton University, Usa
11:00 AM (I)	Catalysis, Energy Storage, and Carbon Capture from a Computational Perspective	De-en	Jiang	ORNL, Oak Ridge, USA
11:30 AM (I)	Advances and Challenges in Computational Catalysis	Lars	Grabow	University of Houston, USA
12:00 PM	Nanoscale metal hydrides for hydrogen storage: effects of size and composition	Lucas	Wagner	University of Illinois, USA
12:20 PM	Cluster Structure Selection Based on Highest Electron Affinity: The Case of TiO <sub>2</sub> Clusters	Noa	Marom	UT-Austin, USA

**Oral Session 1.3.5 Nuclear Materials**  
**Wednesday 2 November: 10:30 am - 12:45 pm (Mountainview B)**  
**Chairperson: Vasily Bulatov**

Time	Title	First Name	Last Name	Affiliation
10:30 AM (I)	Applications of Accelerated Molecular Dynamics in Materials Science	Blas	Uberuaga	Los Alamos National Laboratory, USA
11:00 AM (I)	Self-Evolving Atomistic Kinetic Monte Carlo (SEAK-MC): Development and Application	Haixuan	Xu	ORNL, Oak Ridge, USA
11:30 AM	Influence of alloying of tungsten with transition-metal on dislocation core structure and value of Peierls stress and Peierls potential from first principles	German	Samolyuk	ORNL, Oak Ridge, USA

**Oral Session 2.4 Strongly Correlated Systems and Quantum Phase Transitions**  
**Wednesday 2 November: 10:30 am - 12:45 pm (Gardenview A&B)**  
**Chairperson: Richard Scalettar**

Time	Title	First Name	Last Name	Affiliation
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(I) Invited talk

10:30 AM (I)	Thermodynamics of Strongly Interacting Fermions in 2D Optical Lattices	Marcos	Rigol	Georgetown University, Washington, DC, USA
11:00 AM	An Efficient Quantum Algorithm for Dynamics of a Spin System Coupled to a Spin Bath	Mark A.	Novotny	Mississippi State U, USA
11:20 AM	Thermodynamics and Phase Transitions in the Pinwheel Distorted Kagome Lattice Heisenberg Model	Ehsan	Khatami	Georgetown University, USA
11:40 AM	A theoretical investigation of oxygen vacancy defect in SrTiO <sub>3</sub> , an insulating oxide	Chandrima	Mitra	University of Texas at Austin, USA

**Oral Session 6.1 Plasma Physics**  
**Wednesday 2 November: 10:30 am - 12:45 pm (Mountainview C&D)**  
**Chairperson: Don Batchelor**

Time	Title	First Name	Last Name	Affiliation
10:30 AM (I)	Computational advances in large-scale gyrokinetic particle-in-cell simulations of tokamak fusion devices	Stephane	Ethier	Princeton Plasma Physics Lab, USA
11:00 AM (I)	Fully implicit algorithm for electrostatic PIC simulation of plasmas	Luis	Chacon	ORNL, Oak Ridge, USA
11:30 AM (I)	High-Order Discontinuous Galerkin Schemes with Globally Divergence-Free Constrained Transport for ideal MHD	James	Rossmann	University of Wisconsin - Madison, USA
12:00 PM (I)	Parallel in Time: Trading CPU Cycles for Wall-Clock Time	Lee	Berry	ORNL, Oak Ridge, USA
12:30 PM	Molecular Dynamics Simulations of Dense Plasmas	Andre	da Silva Schnei	Center for Exploration of Energy and Matter and Physics Department - Indiana University, USA

**Oral Session 7.0 Nuclear and High Energy Physics**  
**Wednesday 2 November: 10:30 am - 12:45 pm (Gardenview C&D)**  
**Chairperson: Witold Nazarewicz**

Time	Title	First Name	Last Name	Affiliation
10:30 AM (I)	Real-time calculations of many-body dynamics in quantum systems	Takashi	Nakatsukasa	RIKEN, Japan
11:00 AM (I)	From nucleons to nuclei to fusion reactions	Sofia	Quaglioni	Lawrence Livermore National Laboratory, USA
11:30 AM	Large-Scale Mass table Calculations	Jochen	Erler	Joint Institute of Heavy Ion Research / Physics Division ORNL, Oak Ridge, USA
11:50 AM	Towards a unified description of nuclear structure and reactions with coupled-cluster theory	Gaute	Hagen	ORNL, Oak Ridge, USA
12:10 PM	Charge Radii and Neutron Correlations within the Gamow Shell Model	George	Papadimitriou	University of Tennessee, USA
12:30 PM	UNEDF: Advanced Scientific Computing Collaboration Transforms the Low-Energy Nuclear Many-Body Problem	Hai Ah	Nam	ORNL, Oak Ridge, USA

(I) Invited talk

**Working Lunch**  
**Speaker: G. Malcolm Stocks**  
**"IOP Proceedings Publications"**

**Poster Session 2**  
**Wednesday 2 November: 8:00 - 11:00 pm (Tennessee Ballroom 1)**

Time	Title	First Name	Last Name	Affiliation
P2.1	Theoretical Study of Co/WC Interfaces	Vladlen	Melnikov	Tomsk State University, Russia
P2.2	Decomposition of Neutron Scattering Spectra with Molecular Dynamics Simulations on Dynamics of Cytochrome P450cam	Yinglong	Miao	University of Tennessee/ORNL, Oak Ridge, USA Center for Molecular Biophysics
P2.3	The Solvation Structures of Cellulose Microfibrils in Ionic Liquids	Barmak	Mostofian	University of Tennessee / ORNL, Oak Ridge, USA
P2.4	Retrofit of the HSE density functional	Jonathan	Moussa	Sandia National Labs, USA
P2.5	Effect of the discontinuous wave functions on optimizations of VMC calculations of quantum systems	Amin	Najafi	Department of Physics, Islamic Azad University, Hamedan, Iran
P2.6	The use of atomic level stress to characterize the structure of irradiated iron	Madhu	Ojha	ORNL, Oak Ridge, USA
P2.7	First principles magnetic and electronic structure in large non-periodic dislocation models	Khrgolkhuu	Odbadrakh	ORNL, Oak Ridge, USA
P2.8	Octupole Deformations of Ground State Nuclei	Erik	Olsen	University of Tennessee at Knoxville, USA
P2.9	Fractional quantum Hall effect in systems with band mass anisotropy	Zlatko	Papic	Department of Electrical Engineering, Princeton University, USA
P2.10	Coordinate-space Hartree-Fock-Bogoliubov for Superfluid Fermi Systems in Large Boxes	Junchen	Pei	University of Tennessee/ORNL, Oak Ridge, USA
P2.11	Frozen core method in auxiliary-field quantum Monte Carlo	Wirawan	Purwanto	College of William and Mary, USA
P2.12	Calibrating the Phase-Field Crystal Model for Grain Boundary Motion in Iron	Bala	Radhakrishnan	ORNL, Oak Ridge, USA
P2.13	Thermodynamics of Energy Conversion Devices	David	Rogers	Sandia National Laboratories, USA
P2.14	Simple Heisenberg model based method to accelerate first-principle thermodynamics simulations for magnetic systems	Aurelian	Rusanu	ORNL, Oak Ridge, USA
P2.15	Radical coupling reactions in lignin biosynthesis	Amandeep	Sangha	UT-ORNL, Oak Ridge, USA Center for Molecular Biophysics, USA
P2.16	Crossover phenomena in deterministic and stochastic sandpile models	Sitangshu Bikas	Santra	Department of Physics, Indian Institute of Technology Guwahati, Assam, India

(I) Invited talk

P2.17	Complex States in the Models of Colossal Magnetoresistive Manganites	Cengiz	Sen	University of Tennessee, USA
P2.18	Magnetic properties of the Hubbard model on an fcc lattice	Hao	Shi	College of William and Mary, USA
P2.19	Molecular-Dynamics Study of Crack-Fracture Mechanism by Stealth Dicing	Kohei	Shimamura	Kumamoto University, Japan
P2.20	Stability of Liposome: Free Energy Analysis of Vesicle-to-Bicelle Transformation	Wataru	Shinoda	National Institute of Advanced Industrial Science and Technology, USA
P2.21	Anomalous scaling of moments and multifractality in two-phase flow in porous media	Santanu	Sinha	Norwegian University of Science and Technology, Trondheim, Norway
P2.22	A Coarse-grain model for natural cellulose fibrils	Goundla	Srinivas	ORNL, Oak Ridge, USA
P2.23	Algorithms for quantum cluster simulations with 100+ site clusters	Peter	Staar	ITP ETH Zurich, Switzerland
P2.23	Energy Relaxation Behavior of Optically Generated Hot Carriers in GaN	Kyung Soo	Yi	The Univ. of Texas at Dallas; Pusan National University
P2.24	Towards Modeling Self-Consistent Core Collapse Supernovae	Merek	Chertkow	University of Tennessee, Knoxville, USA
P2.25	Thermonuclear Supernova Simulation: Towards Increased Physical Fidelity to Calibrate the Standard Candle	Suzanne	Parete-Koon	University of Tennessee, Knoxville, USA
P2.26	Numerical Algorithms for Multidimensional Thermonuclear Supernovae Models	Ke-Jung	Chen	University of Minnesota, USA
P2.27	Molecular Dynamics Study on effects of Concentrations of GM1 ganglioside on physical properties of the phospholipid membranes	Daisuke	Takaiwa	National Institute of Advanced Industrial Science and Technology, USA
P2.28	A Parallel Monte Carlo Algorithm For Modeling Dense Stellar Systems On Hybrid Architectures	Bharath	Pattabiraman	Northwestern University, USA

**Plenary VIII AND IX**  
**Thursday 3 November: 8:30, 9:15 Tennessee Ballrooms 3&4)**  
**Chairperson: Tony Mezzacappa**

Time	Title	First Name	Last Name	Affiliation
8:30 AM	Extreme Data-Intensive Scientific Computing	Alex	Szalay	Johns Hopkins Univ., Maryland, USA
9:15 AM	Coupling the Simulation of Electrons with Simulations of Ions	David	Ceperley	Univ. of Illinois, Urbana-Champaign, USA

**Oral Session 1.1.2 Materials /Condensed Matter Theory and Nano Science: General**  
**Thursday 3 November: 10:30 am - 12:45 pm (Mountainview C&D)**  
**Chairperson: Jianxin Zhong**

Time	Title	First Name	Last Name	Affiliation
10:30 AM (I)	Path integral single sweep method for quantum free energy reconstruction	Sara	Bonella	University of Rome, Italy
11:00 AM	Ab initio molecular dynamics simulations of liquid and amorphous silica using Chebyshev-filtered subspace iterations	Minjung	Kim	The University of Texas at Austin, USA
11:20 AM	Correction to the Wills-Harrison approach: Influence on the Fe-based liquid alloys thermodynamics	Nikolay	Dubinin	Russian Academy of Sciences, Ekaterinburg, Russia
11:40 PM	Routines for basic tests of atomistic potentials with universal interface	Bohumir	Jelinek	Mississippi State University, USA
12:00 PM	Ab initio theory of paramagnons in the normal state of unconventional superconductors	Pawel	Buczek	Max Planck Institute of Microstructure Physics, Germany
12:20 PM	Spin waves in the classical Heisenberg antiferromagnet on the Kagome lattice	Stefan	Schnabel	University of Georgia, USA

**Oral Session 1.1.3 Materials /Condensed Matter Theory and Nano Science: General**  
**Thursday 3 November: 10:30 am - 12:45 pm (Gardenview A&B)**  
**Chairperson: M. Claudia Tropicovsky**

Time	Title	First Name	Last Name	Affiliation
10:30 AM (I)	Into the origin of optical activity of carbon nanotubes	Cecilia	Noguez	Universidad Nacional Autonoma, Mexico
11:00 AM (I)	Monte Carlo Simulation of Secondary Electron Emission from Dielectric Targets	Maurizio	Dapor	Fondazione Bruno Kessler, Trento, Italy
11:30 AM (I)	Graphene and its unconventional plasmon properties: A combined theoretical and experimental study	Juan	Idrobo	ORNL, Oak Ridge, USA
12:00 PM	First-principles simulations of exciton diffusion in organic semiconductors	Gang	Lu	California State University Northridge, USA
12:20 PM	The Time Dependent Schrodinger Equation: a multiresolution approach	Nicholas	Vence	University of Tennessee, USA

**Oral Session 5.1 Astrophysics**  
**Thursday 3 November: 11:15 am - 12:45 pm (Gardenview C&D)**  
**Chairperson: Raphael Hix**

Time	Title	First Name	Last Name	Affiliation
11:15 AM (I)	Simulating the Evolution of Galaxies and Clusters of Galaxies	Paul	Ricker	Univ. of Illinois, Urbana-Champaign, USA

(I) Invited talk

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11:45 AM (I)	On Simulating Type Ia Supernovae	Alan	Calder	Stony Brook University, New York, USA
12:15 PM (I)	(Abstract not available)	Bronson	Messer	ORNL, Oak Ridge, USA

**Oral Session 8.1 Complex Systems--Chaos and Statistical Physics**  
**Thursday 3 November: 10:30 am - 12:45 pm (Mountainview B)**  
**Chairperson: Witold Nazarewicz**

Time	Title	First Name	Last Name	Affiliation
10:30 AM (I)	Global Correlation Analysis Based on Optimal Path Identification	Alex	Hansen	Norwegian University of Science and Technology
11:00 AM	Microscopic Dynamics of Ising Spin Glasses in Presence of an External Magnetic Field	Jorge	Monforte	BIFI, Zaragoza, Spain
11:20 AM	Preconditioner methods applied to simulations of two-phase flow in porous media	Morten	Grova	Norwegian University of Science and Technology, Trondheim, Norway
11:40 AM	Numerical simulations of scattering of light from two-dimensional surfaces using the Reduced Rayleigh Equation	Tor	Nordam	Norwegian University of Science and Technology, Trondheim, Norway
12:00 PM	Wang Landau sampling method as a Markov chain	Lev	Shchur	Landau Institute for Theoretical Physics, Moscow, Russia
12:20 PM	Parallelizing the Edward-Anderson spin glass model in Janus, an FPGA based computer	Jose Miguel	Gil Narvion	University of Zaragoza, Spain

**Oral Session 12.3 Computational Physics and Sustainable Energy**  
**Thursday 3 November: 10:30 am - 12:45 pm (Tennessee Ballrooms 3&4)**  
**Chairperson: Bobby Sumpter**

Time	Title	First Name	Last Name	Affiliation
10:30 AM (I)	Theory and microscopy -- complementary tools for energy-related applications	Sok	Pantelides	ORNL, Oak Ridge, USA/Vanderbilt Univ., USA
11:00 AM (I)	Critical Roles of Nanostructures in Hydrogen Storage	Shengbai	Zhang	RPI, Troy, USA
11:20 AM	Influence of the Heat Source Characteristics on Dimensionless Thermal Spreading Resistance	Cui ping	Yan	Beihang University, China
11:40 AM	Predication of 4H-SiC betavoltaics micro battery performance based on a practical Ni-63 source	Gui	Gui	University of Wisconsin-Madison, USA

**Working Lunch**  
**Speaker: Alex Hansen (Norwegian University of Science and Technology)**  
**"CCP 2012 and CCP 2013"**

**Plenary X**  
**Thursday 3 November: 2:15 Tennessee Ballrooms 3&4**  
**Chairperson: Balazs Ujfalussy**

2:15 PM	Petascale High-Fidelity Simulations of Turbulent Reactive Flows: Challenges and Opportunities	Jacqueline	Chen	Sandia National Laboratory, USA
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(I) Invited talk

**Oral Session 1.6.2 Conventional and Order N DFT**  
**Thursday 3 November: 3:15 pm - 5:15 pm (Mountainview C&D)**  
**Chairperson: Paul Kent**

Time	Title	First Name	Last Name	Affiliation
3:15 PM (I)	Pushing some computational limits with all-electron electronic structure theory: Eigenvalue solvers, surface reconstruction, biomolecular structure	Volker	Blum	Fritz Haber Institute of the Max Planck Society, Germany
3:45 PM (I)	Linear-scaling density-functional theory: from fundamental principles to practical applications	Peter	Haynes	Imperial College London, UK
4:15 PM	A Hybrid MPI/OpenMP Implementation for Plane Wave First-principles Materials Science Codes on Multicore Supercomputer Architectures	Andrew	Canning	Lawrence Berkeley National Laboratory and UC Davis, USA
4:35 PM	Exact enumeration of an Ising model for Ni <sub>2</sub> MnGa	Markus	Eisenbach	ORNL, Oak Ridge, USA

**Oral Session 7.1 Nuclear and High Energy Physics**  
**Thursday 3 November: 3:15 pm - 5:15 pm (Mountainview B)**  
**Chairperson: Gaute Hagen**

Time	Title	First Name	Last Name	Affiliation
3:15 PM	Microscopic Calculation of Heavy-Ion Potentials Based on TDHF	Sait	Umar	Vanderbilt University, USA
3:35 PM	Parallel adaptive methods for Feynman loop integrals.	Elise	de Doncker	Western Michigan University, UsA
3:55 PM	Ab Initio Nuclear Structure Calculations of Light Nuclei	Pieter	Maris	Iowa State University, USA

**Oral Session 12.4 Computational Physics and Sustainable Energy**  
**Thursday 3 November: 3:15 pm - 5:15 pm (Tennessee Ballrooms 3&4)**  
**Chairperson: Shengbai Zhang**

Time	Title	First Name	Last Name	Affiliation
3:15 PM (I)	Guiding the Design of Nanostructured Materials for Efficient Energy Storage, Conversion, and Transmission	Bobby	Sumpster	ORNL, Oak Ridge, USA
3:45 PM (I)	Gas Adsorption and Renewable Energy Application: Lesson from Quantum Mechanics	Yong-Hyun	Kim	KAIST, Daejeon, Korea

**Oral Session 5.2 Astrophysics**  
**Thursday 3 November: 3:15 pm - 5:15 pm (Gardenview C&D)**  
**Chairperson: Michael Guidry**

Time	Title	First Name	Last Name	Affiliation
3:15 PM (I)	Turbulent magnetic field amplification from spiral SASI modes in core-collapse	Eirik	Endeve	ORNL, Oak Ridge, USA
3:45 PM (I)	When Black Holes Collide: The Computational Challenge	Pablo	Laguna	Georgia Tech, USA
4:15 PM	Simulations of the First Thermonuclear Supernovae	Ke-Jung	Chen	University of Minnesota, USA
4:35 PM	Molecular dynamics simulations of astrophysical plasma crystals	Charles	Horowitz	Indiana University and ORNL, Oak Ridge, USA

(I) Invited talk

## Alphabetical Author Index

Last Name	First name	Institution	Day	Session ID
Ackland	Graeme	University of Edinburgh, UK	Monday	1.3.1
Adler	Joan	Technion - Israel Institute of Technology	Wednesday	11.1
Ali	Fadhil	Basra University	Monday	P1.1
Alvi	Parvej	Department of Physics, Banasthali University, India	Monday	P1.12
Andersen	Kristopher	High Performance Technologies, Inc.	Monday	1.6.1
Aspuru-Guzik	Alan	Harvard University	Tuesday	1.4.1
Babin	Volodymyr	North Carolina State University	Wednesday	10.3
Baiotti	Luca	Institute of Laser Engineering, Osaka University	Monday	P1.13
Barash	Lev	Landau Institute for Theoretical Physics, 142432, Chernogolovka, Russia	Monday	9.1
Barash	Lev	Landau Institute for Theoretical Physics, Chernogolovka, Russia	Monday	P1.14
Bargoud	George	Pittsburgh Supercomputing Center	Monday	P1.15
Barnard	Amanda	CSIRO Materials Science & Engineering	Wednesday	1.4.3
Berry	Lee	ORNL, Oak Ridge, USA	Wednesday	6.1
Beu	Titus	University Babes-Bolyai, Cluj-Napoca, Romania	Tuesday	1.4.2
Blum	Volker	Fritz Haber Institute of the Max Planck Society	Thursday	1.6.2
Bolhuis	Peter	University of Amsterdam, The Netherlands	Monday	10.1
Bonella	Sara	University of Rome, Italy	Thursday	1.1.2
Buczek	Pawel	Max Planck Institute of Microstructure Physics	Thursday	1.1.2
Bulatov	Vasily	Lawrence Livermore National Laboratory, USA	Monday	1.3.1
Calder	Alan	Stony Brook University, New York, USA	Thursday	5.1
Canning	Andrew	Lawrence Berkeley National Laboratory, UC Davis	Thursday	1.6.2
Carlson	Joseph	Los Alamos National Laboratory, USA	Tuesday	Plenary VI
Ceperley	David	Univ. of Illinois, Urbana-Champaign, USA	Thursday	Plenary IX
Chacon	Luis	ORNL, Oak Ridge, USA	Wednesday	6.1
Chen	Ke-Jung	University of Minnesota	Wednesday	P2.25
Chen	Jacqueline	Sandia National Laboratory, USA	Thursday	Plenary X
Chen	Ke-Jung	University of Minnesota	Thursday	5.2
Chertkow	Merek	University of Tennessee, Knoxville	Wednesday	P2.23
Csanyi	Gabor	Cambridge University, UK	Tuesday	1.5.1
Curtarolo	Stefano	Duke University	Monday	IUPAP YSA
da Silva Schneider	Andre	Center for Exploration of Energy and Matter and Physics Department - Indiana University	Wednesday	6.1
Dapor	Maurizio	Fondazione Bruno Kessler	Thursday	1.1.3
De	Sandip	Department of Physics, Universität Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland	Wednesday	1.4.3
De Decker	Yannick	Université Libre de Bruxelles	Monday	12.1
de Doncker	Elise	Western Michigan University	Thursday	7.1
Demkowicz	Michael	Massachusetts Institute of Technology, USA	Monday	1.3.1
Donev	Aleksandar	New York University	Monday	9.1
Dongarra	Jack	UT/ORNL, Oak Ridge, USA, Knoxville, USA	Monday	Plenary II
Dubin	Nikolay	Institute of Metallurgy of the Ural Branch of the Russian Academy of Sciences, Ekaterinburg, 620016, Russia	Thursday	1.1.2
Dudarev	Sergei	University of Oxford, UK	Monday	1.3.2
Edwards	Robert	Jefferson Lab	Tuesday	4.0
Eisenbach	Markus	ORNL, Oak Ridge, USA	Thursday	1.6.2
El-Mellouhi	Fadwa	Texas A&M University at Qatar	Monday	1.1.1
Endeve	Eirick	ORNL, Oak Ridge, USA	Thursday	5.2
Erler	Jochen	Joint Institute of Heavy Ion Research / Physics Division ORNL, Oak Ridge, USA	Wednesday	7.0
Ethier	Stephane	Princeton Plasma Physics Lab, USA	Wednesday	6.1
Fichthorn	Kristen	Penn State University, USA	Tuesday	1.5.1
Foulkes	William Matthew Colwyn	Imperial College London	Monday	1.7.1
Galloway	Graham	Edinburgh University	Monday	P1.16
Gil Narvion	Jose Miguel	University of Zaragoza	Thursday	8.1
Gjerden	Knut	NTNU	Monday	P1.17

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Last Name	First name	Institution	Day	Session ID
Godoy	William F.	NASA Langley Research Center	Monday	9.1
Golubov	Stanislav	ORNL, Oak Ridge, USA	Monday	1.3.2
Grabow	Lars	University of Houseton, USA	Wednesday	1.2.1
Gross	E.K.U.	Max Planck Institute, Halle, Germany	Monday	Plenary I
Grossman	Jeffery	Massachusetts Institute of Technology, USA	Tuesday	12.2
Grova	Morten	Department of Physics, Norwegian University of Science and Technology (NTNU), NO-7491 Trondheim, Norway	Thursday	8.1
Gui	Gui	University of Wisconsin-Madison	Monday	P1.18
Gui	Gui	University of Wisconsin-Madison	Monday	P1.19
Gui	Gui	University of Wisconsin-Madison	Thursday	12.4
Hagen	Gaute	ORNL, Oak Ridge, USA	Wednesday	7.0
Hansen	Alex	Norwegian University of Science and Technology	Thursday	8.1
Haynes	Peter	Imperial College London, UK	Thursday	1.6.2
Herai	Tomoya	Department of Civil Engineering, Chuo University	Monday	9.1
Herman	Pavel	Faculty of Science, University of Hradec Kralove, Czech Republic	Monday	P1.20
Hong	Liang	Center of molecular biology, ORNL, Oak Ridge, USA	Monday	P1.21
Hood	Randy	Lawrence Livermore National Laboratory, USA	Monday	1.7.2
Horowitz	Charles	Indiana University and ORNL, Oak Ridge, USA	Thursday	5.2
Hu	Shuming	North Carolina State University	Monday	P1.22
Hu	Zixiang	Princeton University	Tuesday	2.1
Hudson	Toby	School of Chemistry, The University of Sydney	Monday	1.1.1
Idrobo	Juan	ORNL, Oak Ridge, USA	Thursday	1.1.3
Iskakova	Kulpash	Rif Akhmaltdinov	Monday	P1.2
Isobe	Masaharu	Nagoya Institute of Technology	Monday	9.1
Ivanov	Ivaylo	Georgia State University, USA	Tuesday	10.2
Jelinek	Bohumir	Mississippi State University	Thursday	1.1.2
Jiang	De-en	ORNL, Oak Ridge, USA	Wednesday	1.2.1
Joo	Balint	Jefferson Lab	Tuesday	4.0
Joshi	Dr. K.B.	Department of Physics, M.L. Sukhadia University, Udaipur-313001, India	Monday	P1.3
Jursenas	Rytis	Institute of Theoretical Physics and Astronomy of Vilnius University, Vilnius, Lithuania	Monday	P1.23
Kaburaki	Hideo	Japan Atomic Energy Agency	Monday	1.1.1
Khatami	Ehsan	Georgetown University, Washington DC	Wednesday	2.4
Kim	Jeongnim	University of Illinois at Urbana-Champaign	Monday	1.7.2
Kim	Kyungsik	Dept. of Physics, Pukyong National University	Monday	P1.4
Kim	Kyungsik	Department of Physics, Pukyong National University	Monday	P1.5
Kim	Minjung	The University of Texas at Austin	Thursday	1.1.2
Kim	Yong-Hyun	KAIST, Daejeon, Korea	Thursday	12.4
Kimizuka	Hajime	Department of Mechanical Science and Bioengineering, Osaka University	Monday	P1.24
Kroegel	Jaron	University of Illinois at Urbana-Champaign	Monday	P1.25
Kuroki	Kazuhiko	The University of Electro-Communications, Japan	Wednesday	2.3
Laguna	Pablo	Georgia Tech, USA	Thursday	5.2
Landau	Rubin H	Oregon State University, USA	Wednesday	11.1
Letnes	Paul Anton	Norwegian University of Science and Technology	Tuesday	1.4.1
Li	Ying Wai	Center for Simulational Physics, University of Georgia, USA	Monday	10.1
Li	Haipeng	City University of Hong Kong, Hong Kong SAR, People's Republic of China.	Monday	P1.6
Lin	Huey-Wen	University of Washington	Wednesday	4.1
Lu	Gang	California State University Northridge	Thursday	1.1.3
Ma	Fengjie	College of William and Mary	Monday	P1.26
Mackenzie	Paul	Fermilab	Tuesday	4.0
Maier	Thomas	ORNL, Oak Ridge, USA	Wednesday	2.3
Marian	Jaime	Lawrence Livermore National Laboratory	Tuesday	1.3.3
Maris	Pieter	Iowa State University	Thursday	7.1
Marom	Noa	UT-Austin	Wednesday	1.2.1
Martin	Richard	Illinois and Stanford, USA	Wednesday	Plenary VII

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Last Name	First name	Institution	Day	Session ID
Marzari	Nicola	University of Oxford, UK	Tuesday	12.2
Mason	Daniel	Imperial College London	Tuesday	1.3.4
Mazzi	Giacomo	Scientific Computing, Dept. Computer Science, K.U. Leuven	Monday	1.1.1
McCaskey	Alexander	ORNL, Oak Ridge, USA (ORNL, Oak Ridge, USA)	Monday	P1.27
Melnikov	Vladlen	Tomsk State University, Russia	Wednesday	P2.1
Messer	Bronson	ORNL, Oak Ridge, USA	Tuesday	Banquet
Messer	Bronson	ORNL, Oak Ridge, USA	Thursday	5.1
Miao	Yinglong	University of Tennessee/ORNL, Oak Ridge, USA Center for Molecular Biophysics	Wednesday	P2.2
Mikame	Shigenori	Department of Civil Engineering, Chuo University	Monday	9.1
Mitas	Lubos	North Carolina State University, USA	Monday	1.7.1
Mitra	Chandrima	University of Texas at Austin	Wednesday	2.4
Monforte	Jorge	BIFI: Instituto de Biocomputaci_n y F_sica de Sistemas Complejos	Thursday	8.1
Moritsugu	Kei	RIKEN, Japan	Monday	10.0
Mostofian	Barmak	University of Tennessee / ORNL, Oak Ridge, USA	Wednesday	P2.3
Moussa	Jonathan	Sandia National Labs	Wednesday	P2.3
Najafi	Amin	Member of department of physic	Wednesday	P2.4
Nakatani	Masahide	Department of Civil Engineering, Chuo University	Monday	1.1.1
Nakatsukasa	Takashi	RIKEN, Japan	Wednesday	7.0
Nam	Hai Ah	ORNL, Oak Ridge, USA	Wednesday	7.0
Negi	Sunita	Sabancı University, Istanbul, Turkey	Tuesday	10.2
Neugebauer	Jorg	Max-Planck-Institut f_r Eisenforschung GmbH	Tuesday	1.5.1
Noguez	Cecilia	Universidad Nacional Autonoma, Mexico	Thursday	1.1.3
Nordam	Tor	Norwegian University of Science and Technology	Thursday	8.1
Novotny	Mark A.	Mississippi State U, USA	Wednesday	2.4
Oberhofer	Harald	TU Munich	Tuesday	12.2
Odbadrakh	Khrgolkhuu	ORNL, Oak Ridge, USA	Wednesday	P2.6
Ohmura	Satoshi	Department of Physics Kumamoto University	Monday	1.1.1
Ojha	Madhu	Oak Ridge National Lab	Wednesday	P2.5
Olsen	Erik	University of Tennessee at Knoxville	Wednesday	P2.7
Orginos	Kostas	College of William & Mary, USA	Tuesday	Plenary IV
Osetskiy	Yury	ORNL, Oak Ridge, USA	Monday	1.3.2
Pantelides	Sok	ORNL, Oak Ridge, USA/Vanderbilt Univ., USA	Thursday	12.3
Papadimitriou	George	University of Tennessee	Wednesday	7.0
Papic	Zlatko	Department of Electrical Engineering, Princeton University	Tuesday	2.2
Papic	Zlatko	Department of Electrical Engineering, Princeton University	Wednesday	P2.8
Pappu	Rohit V.	Washington Univ., Missouri, USA	Tuesday	10.2
Parete-Koon	Suzanne	University of Tennessee, Knoxville	Wednesday	P2.24
Pattabiraman	Bharath	Northwestern University	Wednesday	P2.27
Pattanasiri	Busara	University of Georgia, USA; Mahidol University, Bangkok Thailand	Monday	10.0
Pei	Junchen	University of Tennessee/ORNL, Oak Ridge, USA	Wednesday	P2.9
Peterson	Michael	California State University Long Beach	Tuesday	2.2
Petreczky	Peter	Brookhaven National Lab, USA	Wednesday	4.1
Pine	Polina	Russell Berrie Nanotechnology Institute, Technion	Tuesday	1.4.1
Purwanto	Wirawan	College of William and Mary	Wednesday	P2.10
Qu	Yi-zhi	Graduate University of the Chinese Academy of Sciences, Beijing, China	Thursday	7.1
Quaglioni	Sofia	Lawrence Livermore National Laboratory, USA	Wednesday	7.0
Radhakrishnan	Bala	ORNL, Oak Ridge, USA	Wednesday	P2.11
Regnault	Nicolas	CNRS, Paris, France	Tuesday	2.2
Rezayi	Edward	California State University, Los Angeles	Tuesday	2.1
Richards	David	Jefferson Lab	Tuesday	4.0
Ricker	Paul	Univ. of Illinois, Urbana-Champaign, USA	Thursday	5.1
Rigol	Marcos	Georgetown University, Washington, DC, USA	Wednesday	2.4
Robb	Daniel	Berry College, Georgia, USA	Monday	P1.10
Rogers	David	Sandia National Laboratories	Wednesday	P2.12

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Last Name	First name	Institution	Day	Session ID
Rosmanith	James	University of Wisconsin - Madison	Wednesday	6.1
Rusanu	Aurelian	Oak Ridge National Lab	Wednesday	P2.13
Sakamoto	Shoichi	Seikei University, Japan	Tuesday	1.4.2
Samolyuk	German	ORNL, Oak Ridge, USA	Wednesday	1.3.5
Sangha	Amandeep	UT-ORNL, Oak Ridge, USA Center for Molecular Biophysics	Wednesday	P2.14
Santra	Sitangshu Bikas	Department of Physics, Indian Institute of Technology Guwahati, Assam, India	Wednesday	P2.15
Savage	Martin	University of Washington	Tuesday	4.0
Scalettar	Richard	Univ. of California, Davis, USA	Tuesday	Plenary V
Schnabel	Stefan	University of Georgia	Thursday	1.1.2
Schulthess	Thomas	ETH Zurich	Monday	1.6.1
Selloni	Annabella	Princeton University	Wednesday	1.2.1
Sen	Cengiz	University of Tennessee	Wednesday	P2.16
Sha	Zhendong	Institute of High Performance Computing, Singapore	Monday	P1.7
Shakhnovich	Eugene	Harvard University, USA	Wednesday	10.3
Shchur	Lev	Landau Institute for Theoretical Physics, 142432 Chernogolovka	Thursday	8.1
Shi	Hao	College of William and Mary	Wednesday	P2.17
Shimamura	Kohei	Kumamoto University	Wednesday	P2.18
Shinoda	Wataru	National Institute of Advanced Industrial Science and Technology (AIST)	Wednesday	P2.19
Singh	David	ORNL, Oak Ridge, USA	Monday	12.1
Sinha	Santanu	Norwegian University of Science and Technology, 7491 Trondheim, Norway	Wednesday	P2.20
Smith	Jeremy	ORNL, Oak Ridge, USA	Tuesday	Plenary III
Son	Young-Woo	KIAS, Seoul, Korea	Tuesday	12.2
Sorella	Sandro	Italy	Monday	1.7.2
Srinivas	Goundla	ORNL, Oak Ridge, USA	Wednesday	P2.21
Staar	Peter	ITP ETH Zurich	Wednesday	P2.22
Stoller	Roger	ORNL, Oak Ridge, USA	Tuesday	1.3.3
Sumpter	Bobby	ORNL, Oak Ridge, USA	Thursday	12.4
Szalay	Alex	Johns Hopkins Univ., Maryland, USA	Thursday	Plenary VII
Takaiwa	Daisuke	Nanosystem Research Institute, National Institute of Advanced Industrial Science and Technology (AIST)	Wednesday	P2.26
Tarnavskyy	Oleksandr	Taras Shevchenko National University of Kyiv	Monday	10.1
Torrens	Francisco	Universitat de Valencia-ICMol	Monday	P1.11
Tsuyuki	Hiroyoshi	Seikei University, Japan	Tuesday	1.4.2
Uberuaga	Blas	Los Alamos National Laboratory, USA	Wednesday	1.3.5
Umar	Sait	Vanderbilt University	Thursday	7.1
Valuev	Ilya	Joint Institute for High Temperatures of RAS	Monday	P1.8
Van de Walle	Chris	Materials Department, University of California, Santa Barbara	Monday	12.1
Vence	Nicholas	University of Tennessee	Thursday	1.1.3
Wagner	Lucas	University of Illinois	Wednesday	1.2.1
Wang	Yang	Pittsburgh Supercomputing Center	Monday	P1.9
Weber	William	University of Tennessee	Tuesday	1.3.3
Wosj	Arkadiusz	Wroclaw University, Poland	Tuesday	2.1
Xu	Haixuan	ORNL, Oak Ridge, USA	Wednesday	1.3.5
Yan	Cui ping	Beihang University	Thursday	12.3
Yi	Zheng	ORNL, Oak Ridge, USA/UT Center for Molecular Biophysics	Monday	10.1
Yi	Kyung Soo	The Univ. of Texas at Dallas;Pusan National University	Monday	P1.29
Yi	Kyung Soo	The Univ. of Texas at Dallas;Pusan National University	Wednesday	P2.23
Zeller	Rudolf	Institute of Advanced Simulation, Forschungszentrum Juelich	Monday	1.6.1
Zhang	Shiwei	College of William & Mary	Monday	1.7.1
Zhang	Shengbai	RPI, Troy, USA	Thursday	12.3
Zhong	Jianxin	Xiangtan University, China	Tuesday	1.4.2
Zhou	ShengQuan	University of Illinois at Urbana-Champaign	Monday	P1.28
Zinkle	Steve	ORNL, Oak Ridge, USA	Tuesday	1.3.4

# NOTES

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## Upper Level

<b>Mountainview</b> 100x32 3200 sq. ft. 10' Height Theater 375 Schoolroom 210 Conference 180 Banquet 250			
<b>Moutainview A</b> 20x32 640 sq. ft. 10' Height Theater 75 Schoolroom 42 Conference 36 Banquet 50  <b>A</b>	<b>Moutainview B</b> 40x32 1280 sq. ft. 10' Height Theater 150 Schoolroom 84 Conference 72 Banquet 100  <b>B</b>	<b>Moutainview C</b> 20x32 640 sq. ft. 10' Height Theater 75 Schoolroom 42 Conference 36 Banquet 50  <b>C</b>	<b>Moutainview D</b> 20x32 640 sq. ft. 10' Height Theater 75 Schoolroom 42 Conference 36 Banquet 50  <b>D</b>

<b>Exhibit Hall</b> 20x150 3,000 sq.ft. 10' Height
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## Lower Level

**The LeConte Boardroom**  
640 sq. ft.  
10' Height  
Conference 10  
Additional Perimeter Seating Available

<b>Gardenview</b> Gardenview A&B 40x32 1280 sq. ft. 10' Height Theater 150 Schoolroom 84 Conference 72 Banquet 100		<b>Gardenview</b> Gardenview C,D&E 60x32 1920 sq. ft. 10' Height Theater 225 Schoolroom 126 Conference 108 Banquet 150		
<b>Gardenview A</b> 20x32 640 sq. ft. 10' Height Theater 75 Schoolroom 42 Conference 36 Banquet 50  <b>A</b>	<b>Gardenview B</b> 20x32 640 sq. ft. 10' Height Theater 75 Schoolroom 42 Conference 36 Banquet 50  <b>B</b>	<b>Gardenview C</b> 20x32 640 sq. ft. 10' Height Theater 75 Schoolroom 42 Conference 36 Banquet 50  <b>C</b>	<b>Gardenview D</b> 20x32 640 sq. ft. 10' Height Theater 75 Schoolroom 42 Conference 36 Banquet 50  <b>D</b>	<b>Gardenview E</b> 20x32 640 sq. ft. 10' Height Theater 75 Schoolroom 42 Conference 36 Banquet 50  <b>E</b>

<b>Tennessee Ballroom</b> 74x144 10,656 sq. ft. 23' Height Theater 1500 Schoolroom 1000 Banquet 900			
<b>Tennessee Ballroom 1</b> 36x74 2664 sq. ft. 23' Height Theater 375 Schoolroom 200 Banquet 225  <b>1</b>	<b>Tennessee Ballroom 2</b> 36x74 2664 sq. ft. 23' Height Theater 375 Schoolroom 200 Banquet 225  <b>2</b>	<b>Tennessee Ballroom 3</b> 36x74 2664 sq. ft. 23' Height Theater 375 Schoolroom 200 Banquet 225  <b>3</b>	<b>Tennessee Ballroom 4</b> 36x74 2664 sq. ft. 23' Height Theater 375 Schoolroom 200 Banquet 225  <b>4</b>
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