

54th Sanibel Symposium

February 16-21, 2014

The King and Prince, St. Simons Island, GA



Alternate Plenary Time	Sunday February 16	Time	Monday February 17	Tuesday February 18	Wednesday February 19	Thursday February 20	Friday February 21	
		8:30am to 10:45am	Plenary 3 Stocks <u>X. Zhang</u> M. Eisenbach D. Nicholson D. Johnson	Plenary 7 Butler <u>A. Gupta</u> X. Zhang M. Chshiev D. Stewart	Plenary 10 Öhrn <u>J. Sabin</u> V. Ortiz R. Longo J. Morales	Plenary 13 Schaefer <u>F. Harris</u> D. Yarkony B. Brooks W. Allen	Plenary 15 Bartlett <u>S. Pal</u> J. Stanton M. Nooijen P. Szalay	
		11:05am to 1:00pm	Plenary 4 Young Stars <u>B. Kirtman</u> T. Berlijn C. Cao T. Baruah	Plenary 8 Transport <u>R. Squire</u> K. Park C. Zhang A. Gupta	Plenary 11 Dynamics <u>A. Salam</u> N. Makri N. Ananth G. Cisneros	Plenary 14 Advances in Quantum Chemistry 1 <u>A. Toro-Labbé</u> A. Krylov C. Corminboeuf K. Pernal	Plenary 16 Young Stars <u>M. Musial</u> T. Henderson Á. Szabados A. Beste	
		1:00pm to 2:30pm	FREE TIME					
2:15pm to 4:10pm	Plenary 1 AISEC I <u>K. Runge</u> A. Ng E. Brown J. Kress	2:30pm to 4:25pm	Plenary 5 AISEC III <u>B. Wilson</u> V. Karasiev F. Libisch M.P. Desjarlais	Plenary 9 DFT and applications <u>M. Pederson</u> M. Beltrán M. Fernandez-Serra A. Liu	Plenary 12 Materials Modeling <u>T. Clark</u> S. Staar M. Pederson E. Deumens	Poster 4 <u>G. Shields</u>	Plenary 17 Advances in Quantum Chemistry 2 <u>J. Noga</u> S. Pal M. Gordon V. Kellö	
4:30pm to 6:25pm	Plenary 2 AISEC II <u>R. Magyar</u> T. Sjostrom S. Sorella J. Glosli	4:40pm to 6:35pm	Plenary 6 AISEC IV <u>J. Dufty</u> R. Baer G. Seidler K. Burke	"Beach Discussions"	Poster 3 <u>J. Byrd</u>	Poster 5 <u>D. Lyakh</u>	"Beach Discussions"	
9:00pm to 11:30pm	Reception for Honorees 9:00-10:30pm Delegal Room	9:30pm to 11:30pm	Poster 1 <u>J. Murray</u>	Poster 2 <u>N. Beebe</u>	Symposium Banquet <i>6-pm Cocktails- Patio outside Delegal Room</i> <i>7-10pm Dinner- Delegal Room</i> Lowdin-IBM & Zerner-IBM Awards Poster 1-3 Awards Dell-Intel Awards		Symposium Party 7-10pm Delegal Room Poster 4-6 Awards	

54th Sanibel Symposium



HONORING:

Rod Bartlett

Bill Butler

Yngve Öhrn

Henry Schaefer III

Malcolm Stocks

SPONSORS:

U.S. Department of Energy
Basic Energy Services

Oak Ridge National Laboratory

University of Alabama

University of Georgia

University of Florida
Office of Research
College of Liberal Arts & Sciences
Department of Chemistry
Department of Physics
Quantum Theory Project

AWARDS:

Dell-Intel

IBM

February 16-21, 2014 - The King and Prince, St. Simons Island, GA



TABLE OF CONTENTS



Plenary Session Schedule	Inside Front Cover
Welcome	4
Honorees	5
Registration Desk Hours	6
Procedures & Practical Matters	6
Assistance	6
Social Activities	6
Poster Session Instructions	7
Proceedings Contribution Instructions	7
Plenary Session Instructions	7
Sanibel Symposium Staff	8
Donor Information	8
Donors	9

PROGRAM

All Plenary Sessions will be held in the Lanier Ballroom. All Poster Sessions will begin with 2-minute introductions in the Lanier Ballroom, followed by displays in the Retreat Room.

Sunday, February 16

Plenary 1- Ab Initio Simulations at Extreme Conditions I	10
Plenary 2- Ab Initio Simulations at Extreme Conditions II	10

Reception for Honorees
Delegal Room 9:00-10:30pm
Two drink tickets provided

Monday, February 16

Plenary 3- Stocks	10
Plenary 4- Young Stars	11
Plenary 5- Ab Initio Simulations at Extreme Conditions III	11
Plenary 6- Ab Initio Simulations at Extreme Conditions IV	11
Poster 1	12

Tuesday, February 17

Plenary 7- Butler	13
Plenary 8- Transport	14
Plenary 9- DFT and Applications	14
Poster 2	14



TABLE OF CONTENTS



Wednesday, February 18

Plenary 10- Öhrn	16
Plenary 11- Dynamics	16
Plenary 12- Materials Modeling	16
Poster 3	17

Symposium Banquet

6:00-7:00pm- Cocktail Hour - Delegal Room Patio (weather permitting)

7:00-10:00pm- Banquet Dinner- Delegal Room

Ticket required

Thursday, February 20

Plenary 13- Schaefer	19
Plenary 14- Advances in Quantum Chemistry 1	19
Poster 4	19
Poster 5	20

Friday, February 21

Plenary 15- Bartlett	21
Plenary 16- Young Stars	22
Plenary 17- Advances in Quantum Chemistry 2	22

Symposium Party

7:00-10:00pm- Delegal Room

Ticket required

List of Participants

23

Poster Session Schedule

Inside Back Cover



WELCOME



Welcome to the 54th Sanibel Symposium! We hope you find the scientific program rich and valuable and that you will benefit from personal discussions with other leading scientists in quantum chemistry, theoretical and computational materials physics, and chemical physics.

This year's meeting recognizes five leaders in our field: Bill Butler, Yngve Öhrn, Henry Schaefer III, Malcolm Stocks and Rod Bartlett. The 17 Plenary Session topics were chosen by the organizers to have two focus areas. The first is a 4-session sub-symposium on *ab initio* simulations of systems under extreme conditions. The second is the 8-session "360-view" sub-symposium which honors those five leaders in the broad area of quantum chemistry and materials physics. The remaining 5 plenary sessions cover a selection of other current topics. The Symposia have their own special character that have their roots in the original Sanibel Island meetings. As always, we appreciate suggestions for Plenary Session topics and ways to improve the Sanibel Symposium.

We are pleased to acknowledge the sponsors of the 54th Sanibel Symposium. Thanks to the generous contributions from our sponsors, we are pleased to award competitive stipends to support participation in the Symposium.

For the 54th Sanibel Symposium, we have received support from:

U.S. Department of Energy
Basic Energy Services

Oak Ridge National Laboratory

University of Alabama

University of Georgia

University of Florida
Office of Research
College of Liberal Arts & Sciences
Department of Chemistry
Department of Physics
Quantum Theory Project

AWARDS:

Dell-Intel

IBM

PROCEEDINGS PUBLISHER:

Taylor and Francis



Sanibel Award - Outstanding QTP Graduate Student 2013
Dr. Robert Molt.

54th Sanibel Symposium

Honorees



Rod Bartlett

Graduate Research Professor, Quantum Theory Project, University of Florida

Pioneered the development of coupled-cluster theory in quantum chemistry to offer highly accurate determinations of molecular structure and spectra.



Bill Butler

Director, Center for Materials and Information Technology, Professor Physics and Astronomy, University of Alabama

Led breakthroughs in transport theory of metals, alloys, and tunnel junctions, in particular the understanding of the giant magnetoresistance in magnetic multilayers and the prediction of giant tunneling magnetoresistance in magnetic tunnel junctions



Yngve Öhrn

Professor of Chemistry and Physics, Quantum Theory Project, University of Florida

Pioneered the use of propagators in molecular quantum mechanics, and he together with Erik Deumens, developed and applied a time-dependent, direct, non-adiabatic theory, called END, for reactive molecular processes.



Henry F. Schaefer III

Graham Perdue Professor of Chemistry and Director of the Center for Computational Chemistry at the University of Georgia

Developed and applied quantum chemical methods to describe and understand the movement of electrons in molecules and its application to a broad array of problems of chemical interest. He has been a professor of theoretical chemistry for 45 years, 18 at Berkeley and now 27 years at Georgia.



Malcolm Stocks

Corporate Fellow, Group Leader for Materials Theory, Oak Ridge National Laboratory

Pioneered massively parallel computing for first-principles electronic structure calculations, led the world in fastest scientific computing applications multiple times, and made seminal contributions to theories of alloy phase stability and magnetic materials.

Poster 1 Monday February 17 9:30-11:30pm Jane Murray Chair	Poster 2 Tuesday February 18 9:30-11:30pm Nelson Beebe Chair	Poster 3 Wednesday February 19 4:40-6:35pm Jason Byrd Chair	Poster 4 Thursday February 20 2:30-4:25pm George Shields Chair	Poster 5 Thursday February 20 4:40-6:35pm Dmitry Lyakh Chair
<ol style="list-style-type: none"> 1. Andrew Baczewski 2. Mandy Bethkenhagen 3. Chris Billman 4. Florent Calvayrac 5. Gloria Cardenas-Jiron 6. Debajit Chakraborty 7. James Dufty 8. Boris Galabov 9. Rashid Hamdan 10. Yulun Han 11. Thomas Jagau 12. Dmitri Kilin 13. Svetlana Kilina 14. Shubin Liu 15. Eyal Segev 16. Masako Takasu 17. Jonathan Trinastic 18. Nicolas Vinson 19. Yun-Peng Wang 20. Tomonori Yamada 21. Long Zhang 	<ol style="list-style-type: none"> 1. Yusuke Asari 2. Antonio Cancio 3. Iek-Heng Chu 4. Tania Cordova-Sinjago 5. Alfredo Correa 6. Marta Dudek 7. Tomoyuki Hamada 8. Yulun Han 9. Shuping Huang 10. Benjamin Janesko 11. Stephanie Jensen 12. Xiangguo Li 13. Sahar Mirshamsi 14. Jeffery Mottishaw 15. Monika Musial 16. Wendi Sapp & Adam Erck 17. Paul Seybold 18. Juliusz Stasiewicz 19. Yu Takano 20. Dayton Jonathan Vogel 21. Chia-Hua Wu 22. Ge Yao 	<ol style="list-style-type: none"> 1. Atanu Acharya 2. Arie Aizman 3. Hiroyuki Ando 4. Naveen Dandu 5. Xintian Feng 6. Matthew Hermes 7. Youqi Ke 8. Dmitry Lyakh 9. Jane Murray 10. Ryota Nakamura 11. Akisumi Okamoto 12. Ajith Perera 13. Frank Pickard 14. Austin Privett 15. Hiroaki Saito 16. Akbar Salam 17. Richard Squire 18. Teresa Tamayo-Mendoza 19. Steven Wheeler 20. Junchao Xia 21. Daisuke Yamaki 22. Shusuke Yamanaka 23. Takehiro Yonehara 24. Yuchi Zhang 	<ol style="list-style-type: none"> 1. Alexandre Bazanté 2. Denis Bokhan 3. Peter Langhoff 4. Svetlana Malinovskaya 5. Vladimir Malinovsky 6. Jozef Noga 7. Marie V. Parkes 8. James J. Shepherd 9. Tamar Stein 10. Brian Wilson 	<ol style="list-style-type: none"> 1. Jason Byrd 2. Tania Cordova-Sintjago 3. Tania Cordova-Sintjago 4. Mohammad H. Hasan 5. Robert H. Hembree 6. John Mintmire 7. Takeshi Miyakawa 8. Jose Juan Peña 9. Scott Rabidoux 10. Jules Tshishimbi Muya 11. Kizashi Yamaguchi



PARTICIPANTS



Alexandre Patrick Bazanté
University of Florida
Quantum Theory Project
2330 SW Williston Rd.
3114
Gainesville FL 32608
United States
(352) 213-7595
alexandrebazante@gmail.com

Nelson H F Beebe
Research Professor of Mathematics
University of Utah
Department of Mathematics, 110 Lcb
155 S. 1400 E. Rm 233
Salt Lake City UT 84112-0090
United States
(801) 581-5254
(801) 581-4148
beebe@math.utah.edu

Marcela Regina Beltrán
Prof.
Universidad Nacional Autónoma de México
Circuito Exterior S./N. Ciudad Universitaria
Apartado Postal 70-360
Ciudad Unversitaria Delegacion Coyoacán.
Cde De Mexico D.f. 04510
Mexico
+52 55-56224624
+52 55-56221251
mbeltran@unam.mx

Tom Berlijn
Oak Ridge National Laboratory
10121 Wolf Den Ln.
Knoxville TN 37932
United States
(631) 356-3062
tberlijn@gmail.com

Ariana Beste
Research Scientist
University of Tennessee
1 Bethel Valley Rd.
PO Box 2008, MS 6211
Oak Ridge TN 37831
United States
(865) 241-3160
bestea@ornl.gov

Mandy Bethkenhagen
University of Rostock
Wismarsche Str. 43-45
Rostock M-V 18057
Germany
mandy.bethkenhagen@uni-rostock.de

Chris Billman
Graduate Student
University of Florida
328 SW 34th St.
5
Gainesville FL 32607
United States
billman@phys.ufl.edu

Denis Bokhan
Research Associate
Moscow State University
914 SW 8th Ave., Unit #37
Gainesville FL 32601
United States
denisbokhan@mail.ru

Bernard Brooks
Chief
Laboratory of Computational Biology
5635 Fishers Ln.
Ste. T-900
Rockville MD 20852
United States
brb@mail.nih.gov

Ethan W. Brown
Graduate Researcher
University of Illinois / Lawrence Livermore National Laboratory
405 Bellevue Ave.
306
Oakland CA 94610
United States
(918) 520-9342
ethan.w.brown@gmail.com



PARTICIPANTS



Kieron Burke
Professor
University of California, Irvine
1102 Natural Sciences
Irvine CA 926972025
United States
(949) 824-0374
kieron@uci.edu

Jason N. Byrd
Postdoctoral Associate
University of Florida
Quantum Theory Project
700 SW 62nd Blvd. G88
2152 Hillside Rd.
Gainesville FL 32607
United States
(860) 402-4933
byrdja@chem.ufl.edu

Florent S. Calvayrac
Université du Maine (Le Mans)
IMMM/ Faculté des Sciences et Techniques
Ave. Olivier Messiaen
Université du Maine
Le Mans 72085
France, Metropolitan
+33 6-64314386
+33 2-43833518
florent.calvayrac@univ-lemans.fr

Antonio C. Cancio
Ball State University
Department of Physics and Astronomy
2000 W. University Ave.
Ball State University
Muncie IN 47306
United States
(765) 285-8868
accancio@bsu.edu

Chao Cao
Professor
Hangzhou Normal University
No. 16 Xuelin St.
College of Science
Hangzhou Zhejiang 310036
China, Peoples Republic of
+86 571-28860503 ext. 803
ccao@hznu.edu.cn

Gloria Cardenas-Jiron
Universidad de Santiago de Chile (USACH)
Av. Bernardo O'Higgins 3363
Santiago
Chile
gloria.cardenas@usach.cl

Debajit Chakraborty
Post Doctoral Associate
University of Florida
Quantum Theory Project
QTP, Room NO: 2302
Department of Physics
University of Florida
Gainesville FL 32611
United States
(352) 263-4191
(352) 263-4191
deb.chakraborty@ufl.edu

Daniel Chaves Claudino
University of Florida
3461 SW 2nd Ave. # 248
Gainesville FL 32607
United States
(352) 727-1319
dclaudino@ufl.edu

Hai-Ping Cheng
Professor of Physics and Qtp
University of Florida
2330 NPB Dept. of Physics
Gainesville FL 32611
United States
(352) 392-6256
(352) 392-8722
cheng@qtp.ufl.edu

Mairbek Chshiev
SPINTEC, CEA/CNRS/UJF-Grenoble
17 Rue Des Martyrs
Grenoble 38054
France
mair.chshiev@cea.fr



PARTICIPANTS

**Iek-Heng Chu**

Graduate Student
University of Florida
385 Maguire Vlg, # 6
Gainesville FL 32603
United States
(352) 213-7856
johns866@ufl.edu

Gerardo Andrés Cisneros

Wayne State University
5101 Cass Ave.
Detroit MI 48202
United States
(313) 577-2571
andres@chem.wayne.edu

Tim Clark

Professor
University of Erlangen
Computer-Chemie-Centrum
Naegelsbachstr. 25
Erlangen 91052
Germany
+49 9131-8522948
+49 9131-8526565
tim.clark@fau.de

Tania Cordova-Sintjago

University of Florida
1600 SW Archer Rd.
Gainesville FL 32610
United States
(352) 352-2737
taniacsintjago@yahoo.com

Clémence Corminboeuf

Professor
École Polytechnique Fédérale de Lausanne
EPFL-SB-ISIC-Batochime
BCH 5312
Lausanne Vaud 1015
Switzerland
clemence.corminboeuf@epfl.ch

Alfredo A. Correa

Staff
Lawrence Livermore National Laboratory
7000 E. Ave.
Livermore CA 94550
United States
(650) 918-6159
correaa@llnl.gov

Naveen Kumar Dandu

Chemistry Graduate Student
North Dakota State University
Department of Chemistry and Biochemistry
177 University Vlg
Fargo ND 58102
United States
(701) 205-2929
(701) 231-8831
naveen.dandu@my.ndsu.edu

Michael Desjarlais

Sandia National Laboratories
14000 Villa Sandia Pl. NE
Albuquerque NM 87112
United States
(505) 228-6501
mpdesja@sandia.gov

Erik Deumens

Director
University of Florida
NPB 2334
2001 Museum Rd.
University of Florida
Gainesville FL 32611-8435
United States
(352) 392-6980
deumens@ufl.edu

James W. Dufty

Professor
University of Florida
Department of Physics
PO Box 118440
Gainesville FL 32611
United States
(352) 262-2112
dufty@phys.ufl.edu



PARTICIPANTS



Markus Eisenbach
Oak Ridge National Laboratory
One Bethel Valley Rd.
Oak Ridge TN 37831
United States
(865) 924-0910
eisenbachm@ornl.gov

Adam R. Erck
University of South Dakota
411 Stanford, #8
Vermillion SD 57069
United States
(605) 929-2552
adam.erck@usd.edu

Xintian Feng
University of Southern California
Ssc 417
University of Southern California
Los Angeles CA 90089
United States
(213) 309-5855
xintianf@usc.edu

Marivi Fernandez-Serra
Associate Professor
Stony Brook University
Physics Department
Stony Brook NY 11733
United States
maria.fernandez-serra@stonybrook.edu

Boris S. Galabov
Visiting Research Professor
University of Georgia
Center for Computational Quantum Chemistry
1004 Cedar St., Room 505
Athens GA 30602
United States
(706) 542-0364
(706) 542-0406
ohtbg@wmail.chem.uni-sofia.bg

James Glosli
Physicist
Lawrence Livermore National Laboratory
P.O Box 808 L367
Livermore CA 94550
United States
(925) 422-5849
glosli@llnl.gov

Mark Gordon
Distinguished Professor of Chemistry
Iowa State University
201 Spedding Hall
Ames IA 50011
United States
(515) 294-0452
mark@si.msg.chem.iastate.edu

Arunava Gupta
Professor
University of Alabama
2007 Beville Building
Mint Center
Tuscaloosa AL 35487
United States
(205) 348-3822
(205) 348-2346
agupta@mint.ua.edu

Soledad Gutiérrez-Oliva
Dr
Pontificia Universidad Católica de Chile
Av Vicuña Mackenna 4860
Macul
Santiago
Chile
56 22354143
msg@uc.cl

Tomoyuki Hamada
Chief Researcher
Hitachi, Ltd.
Central Research Laboratory, Hitachi Ltd.
Hatoyama Saitama 350-0395
Japan
+81 49-2966111
+91 49-2966005
tomoyuki.hamada.tk@hitachi.com



PARTICIPANTS



Rashid Hamdan
University of Florida
Dept of Physics
New Physics Bldg
Gainesville FL 32611
United States
(352) 871-6609
rashidhamdan@gmail.com

Yulun Han
University of South Dakota
1014 Elm St. #. 203
Vermillion SD 57069
United States
yulun.han@coyotes.usd.edu

Frank Harris
Adjunct Professor
University of Florida
Quantum Theory Project
PO Box 118435
Gainesville FL 32611
United States
(352) 392-6975
harris@qtp.ufl.edu

Mohammad H. Hasan
Professor
Kuwait University
Chemistry Department
P. O. Box 5969
Safat Safat 13060
Kuwait
(965) 996-8694 5
965 2-4826482
m.hasan@ku.edu.kw

Robert H. Hembree
Graduate Student
University of Florida
Quantum Theory Project
3801 SW 13th St.
202d
Gainesville FL 32608
United States
(434) 851-5113
rhembree@ufl.edu

Thomas M. Henderson
Research Associate
Rice University
Department of Chemistry
6100 Main St.
Houston TX 77005
United States
th4@rice.edu

Matthew R. Hermes
Research Assistant
University of Illinois at Urbana-Champaign
600 S. Mathews Ave.
Box 83-6
Urbana IL 61801
United States
(651) 357-0613
hermes6@illinois.edu

Shuping Huang
Postdoctoral Reseacher
University of South Dakota
530 Elm St. # 28
Vermillion SD 57069
United States
huangshp@gmail.com

Thomas Christian Jagau
University of Southern California
3620 McClintock Ave.
SSC 411
Los Angeles CA 90089
United States
(213) 740-0893
jagau@usc.edu

Benjamin G. Janesko
Assistant Professor
Texas Christian University
2800 S. University Dr. Box 298860
Fort Worth TX 76109
United States
b.janesko@tcu.edu



PARTICIPANTS



Stephanie Jean Jensen
University of South Dakota
709 Tom St.
Vermillion SD 57069
United States
(605) 670-7674
stephanie.reed@usd.edu

Yifan Jin
281 Corry Village # 8
Gainesville FL 32603
United States
(352) 213-3387
yjin@chem.ufl.edu

Duane Johnson
Chief Research Officer
Ames Laboratory
311 Tasf
Ames Laboratory/ISU
Ames IA 50011
United States
(515) 294-2770
ddj@ameslab.gov

Valentin Karasiev
Dr
University of Florida
Quantum Theory Project
PO Box 118435
Gainesville FL 32611-8435
United States
(352) 392-6976
vkarasev@qtp.ufl.edu

Youqi Ke
Postdoctoral Associate
Princeton University
D324 Equad
Olden St.
Princeton NJ 08544
United States
(609) 258-1914
yke@princeton.edu

Vladimir Kellö
Professor
Comenius University
Dept. of Phys. and Theoret. Chem.
Faculty of Natural Sciences, Comenius University
Mlynska Dolina Ch-1
Bratislava Sk-84215
Slovak Republic
+421 2-60296553
+421 2-60296231
kelloe@fns.uniba.sk

Dmitri Kilin
University of South Dakota
Department of Chemistry
414 E. Clark St.
Vermillion SD 57069
United States
(206) 356-2212
dmitri.kilin@usd.edu

Svetlana Kilina
Assistant Professor
North Dakota State University
Po Box 6050
Department of Chemistry and Biochemistry
 Fargo ND 58108-6050
United States
(206) 529-7174
svetlana.kilina@ndsu.edu

Bernard Kirtman
Professor
University of California Santa Barbara
Department of Chemistry & Biochemistry
Santa Barbara CA 93106-9510
United States
(805) 893-2217
(805) 893-4120
kirtman@chem.ucsb.edu

Joel D. Kress
Group Leader
Los Alamos National Laboratory
Group T-1, Mail Stop B221
Los Alamos NM 87544
United States
(505) 667-8906
jdk@lanl.gov



PARTICIPANTS

**Anna Krylov**

University of Southern California
Dept. of Chemistry
USC
Los Angeles CA 91103
United States
krylov@usc.edu

Peter W. Langhoff

Senior Faculty Affiliate
University of California- San Diego
5332 Renaissance Ave.
San Diego CA 92122
United States
(858) 822-3611
(858) 534-4974
langhoff@drifter.sdsc.edu

Xiangguo Li

Graduate Student
University of Florida
393 Maguire Village # 3
Gainesville FL 32603
United States
(352) 665-1934
li@phys.ufl.edu

Florian Libisch

Vienna University of Technology
Wiedner Hauptstraße. 8-10
Vienna Vienna 1040
Austria
43 1-58801 ext. 13608
fortran.flo@gmail.com

Amy Liu

Professor
Georgetown University
Department of Physics, 506 Reiss
Georgetown University
Washington DC 20057
United States
liu@physics.georgetown.edu

Shubin Liu

Senior Computational Scientist
University of North Carolina
Research Computing Center
105 Telluride Trail
Chapel Hill NC 27514
United States
(919) 962-4032
(919) 962-0417
shubin@email.unc.edu

Ricardo Luiz Longo

Professor
Universidade Federal de Pernambuco
Rua Jader De Andrade, 404 - # 1201
Casa Forte
Recife PE 52061-060
Brazil
+55 81-21268459
+55 81-21268442
longo@ufpe.br

Dmitry I. Lyakh

University of Florida
Quantum Theory Project
2001 Museum Rd., Ofc. 2319
Gainesville FL 32611
United States
quant4me@gmail.com

Rudolph J. Magyar

Senior Member of the Technical Staff
Sandia National Laboratories
Po Box 5800, Ms 1322
Ms 1322
Albuquerque NM 87113
United States
(505) 930-0718
(505) 284-2518
rjmagya@sandia.gov

Nancy Makri

Professor
University of Illinois
600 S. Goodwin Ave.
Champaign IL 61822
United States
(217) 333-6589
nmakri@illinois.edu



PARTICIPANTS

**Svetlana A. Malinovskaya**

Associate Professor
Stevens Institute of Technology
Department of Physics and Engineering Physics
Castle Point on Hudson
Hoboken NJ 07013
United States
(201) 216-8094
smalinov@stevens.edu

Vladimir S. Malinovsky

US Army Research Laboratory
2800 Powder Mill Rd.
Adelphi MD 20783
United States
(734) 657-5391
vsmalinovsky@gmail.com

David A. Micha

Professor (Adj, Emr)
University of Florida
Quantum Theory Project
2318 NPBldg
POB 118435
University of Florida
Gainesville FL 32611
United States
(352) 392-6977
(352) 392-4310
micha@qtp.ufl.edu

John W. Mintmire

Regents Professor and Head
Oklahoma State University
1906 S. Iba Dr.
Oklahoma State University
Stillwater OK 74074-1332
United States
(405) 377-5390
(405) 744-6811
john.mintmire@okstate.edu

Sahar Mirshamsi

Graduate Student
University of Florida
Quantum Theory Project
3901 SW 20th ave
Gainesville FL 32607
United States
(352) 872-8590
smirshamsi@phys.ufl.edu

Takeshi Miyakawa

Assistant Professor
Tokyo University of Pharmacy and Life Sciences
School of Life Sciences
1432-1 Horinouchi
Hachioji Tokyo 192-0392
Japan
81 042-6764561
81 042-6764561
takeshi@toyaku.ac.jp

Jorge Alberto Morales

Associate Professor
Texas Tech University
Department of Chemistry and Biochemistry
Memorial Cir. & Boston
Lubbock TX 79409
United States
(806) 834-3094
jorge.morales@ttu.edu

Jeffery Dale Mottishaw

Research Assistant/Doctoral Candidate
University of South Dakota
Churchill-Haines Laboratories Room 115
University of S. Dakota
414 E. Clark St.
Vermillion SD 57069
United States
(208) 380-9229
jeffmottishaw@gmail.com

Jane S. Murray

Researcher
University of New Orleans
18860 Timber Ln.
Fairview Park OH 44126
United States
(202) 351-1554
jsmurray@uno.edu

Monika Musial

University of Silesia
Szkolna 9
Institute of Chemistry
Katowice Silesia 40-006
Poland
48 32359 ext. 1675
musial@ich.us.edu.pl



PARTICIPANTS



Ryota Nakamura
Graduate School Student
Osaka University
Machikaneyama-Cho 1-3
Toyonaka Osaka 560-8531
Japan
+81 6-6850 ext. 6265
ryotin0926@gmail.com

Andrew Ng
Professor Emeritus
University of British Columbia
Department of Physics and Astronomy
6224 Agricultural Road
Vancouver V6T 1Z1
Canada
nga@physics.ubc.ca

Don Nicholson
Oak Ridge National Laboratory
224 Connors Cir.
Oak Ridge TN 37830
United States
(865) 253-6922
dnicholson.or@gmail.com

Jozef Noga
Comenius University
Faculty of Natural Sciences, Bratislava
Mlynska Dolina CH2
Bratislava 81108
Slovak Republic
jozef.noga@fns.uniba.sk

Marcel A. Nooijen
Dr.
University of Waterloo
200 University Ave. W.
University of Waterloo
Department of Chemistry
Waterloo ON N2L 3G1
Canada
(519) 888-4567 ext. 37708
nooijen@uwaterloo.ca

Yngve Öhrn
Professor
University of Florida
1823 NW 11th Rd.
Gainesville FL 32605
United States
(352) 328-4059
ohrn@qtp.ufl.edu

Akisumi Okamoto
Toyohashi University of Technology
1-1 Hibarigaoka, Tempaku
Toyohashi, Aichi Aichi 441-8580
Japan
81 53244657
okamoto@klab.cs.tut.ac.jp

Vincent Ortiz
Molette Professor and Chairman
Auburn University
179 Chemistry Building
Auburn AL 36849-5312
United States
(334) 844-4043
(334) 844-6959
ortiz@auburn.edu

Kyungwha Park
Virginia Tech
Dept of Physics, Robeson Hall
MC0435, 850 West Campus Drive
Blacksburg VA 24061
United States
(540) 231-5533
kyungwha@vt.edu

Marie V. Parkes
Postdoctoral Appointee
Sandia National Laboratories
13309 Indian School Rd. NE
Albuquerque NM 87112
United States
(505) 681-5082
mvparke@sandia.gov



PARTICIPANTS



Mark R. Pederson
Program Manager
U.S. Department of Energy
19901 Germantown Rd., Room E.-433
Germantown MD 20874-1920
United States
(202) 422-4814
mark.pederson@science.doe.gov

Jose Juan Peña
Universidad Autónoma Metropolitana Azc.
San Pablo 180. Col. Reynosa, Azc.
Reynosa Azcapotzalco
Mexico Df D.f 02200
Mexico
+0052 55-53189575
jjpg@correo.azc.uam.mx

Ajith D. Perera
Associate Scientist
University of Florida
Department of Chemistry
University of Florida
Gainesville FL 32611
United States
(352) 392-6616
perera.ajith@gmail.com

Katarzyna Pernal
Lodz University of Technology
Ul. Wolczanska 219
Lodz 90-924
Poland
+48 42-6313656
pernalk@gmail.com

Frank Clemence Pickard
IRTA Post Doctoral Fellow
National Institutes of Health
6030 California Cir.
207
Rockville MD 20852
United States
(301) 541-3371
pickard81@gmail.com

Peter Politzer
Boyd Professor Emeritus
University of New Orleans
18860 Timber Ln.
Fairview Park OH 44126
United States
(202) 351-1555
ppolitze@uno.edu

Austin J. Privett
Graduate Student
Texas Tech University
5302 11th St. #218
Lubbock TX 79416
United States
austin.privett@ttu.edu

Scott M. Rabidoux
University of Texas - Austin
612 W. N. Loop Blvd.
A
Austin TX 78751
United States
(859) 802-0356
scottrabidoux@gmail.com

Karnamohit Ajit Ranka
Graduate Student
University of Florida
NPB 2224, Physics building
2001 Museum Road
University of Florida
Gainesville FL 32611
United States
(352) 870-5456
kmrk24@ufl.edu

Varun Rishi
University of Florida
Quantum Theory Project
278 Corry Vlg # 7
Gainesville FL 326032137
United States
(352) 870-6642
varunrishi@ufl.edu



PARTICIPANTS



Adrian E Roitberg
University of Florida
LEI Hall #400
University of Florida
Department of Chemistry
Gainesville FL 32611-7200
United States
(352) 392-6972
roitberg@ufl.edu

John Rogers Sabin
University of Florida
Quantum Theory Project
Po Box 118435
University of Florida
Gainesville FL 32611-8435
United States
(352) 392-1597
sabin@qtp.ufl.edu

Wendi Sapp
University of South Dakota
411 Sanford, #8
Vermillion SD 57069
United States
(605) 659-4924
wendi.sapp@coyotes.usd.edu

Gerald Seidler
Professor
University of Washington
Physics, Box 351560
University of Washington
Seattle WA 98195-1560
United States
(206) 427-8045
seidler@uw.edu

James John Shepherd
Rice University
6100 Main St.
Houston TX 77005
United States
(832) 209-9950
jjs6@rice.edu

Keith Runge
Adjunct Professor
University of Florida
Quantum Theory Project
2901 NW 54th Ave.
Gainesville FL 32653
United States
(352) 367-1461
krunge@ufl.edu

Hiroaki Saito
Kanazawa University
Kakuma
Kanazawa Ishikawa 920-1192
Japan
hiroaki.saito.daimei@gmail.com

Henry F. Schaefer III
Director and Graham Professor of Chemistry
University of Georgia
The Center for Computational Chemistry
University of Georgia
1004 Cedar St., Room 505
Athens GA 30602
United States
(706) 542-0364
(706) 542-0406
qc@uga.edu

Paul G. Seybold
Prof.
Wright State University
Chemistry Department
3640 Col. Glenn Hwy.
Chemistry Department
Wright State University
Dayton OH 45435
United States
(937) 775-2407
(937) 775-2717
paul.seybold@wright.edu

George C. Shields
Dean of Arts & Sciences
Bucknell University
College of Arts and Sciences
Dent Dr.
Lewisburg PA 17837
United States
(570) 577-3292
george.shields@bucknell.edu



PARTICIPANTS



Travis Sjostrom
Postdoctoral Associate
Los Alamos National Lab
Quantum Theory Project
3200 Canyon Rd. #3306
Los Alamos NM 87544
United States
(801) 628-6571
sjostrom@lanl.gov

Sandro Sorella
Professor
Scuola Internazionale Superiore di Studi Avanzati
SISSA
Via Bonomea N.265
Trieste Friuli Venezia Giulia 34136
Italy
+39 040-3787 ext. 444
+39 040-3787 ext. 528
sorella@sissa.it

Richard Squire
Associate Professor
West Virginia University - Institute of Technology
405 Fayette Pike
Montgomery WV 25136
United States
(304) 744-2903
richard.squire@mail.wvu.edu

Peter Staar
ETH Zurich
Wolfgang-Pauli-Str. 27
8093 Zurich, Switzerland
Zurich Zurich 8093
Switzerland
staarp@itp.phys.ethz.ch

John F. Stanton
University of Texas- Austin
6011 Back Bay Ln.
Austin TX 78739
United States
(512) 293-9622
jfstanton@mail.utexas.edu

Juliusz Stasiewicz
International Institute of Molecular and Cell Biology in
Warsaw
Ks. Trojdena 4
Warsaw 02-109
Poland
jstasiewicz@genesilico.pl

Derek Stewart
Cornell University
250 Duffield Hall
Cornell University
Ithaca NY 14853
United States
(607) 255-2856
derek.stewart@cornell.edu

G. Malcolm Stocks
Corporate Fellow
Oak Ridge National Laboratory
PO Box 2008-6114
Oak Ridge TN 37830
United States
(865) 574-5163
stocksgm@ornl.gov

Ágnes Szabados
Eötvös Loránd University
1/A Pázmány Péter Sétány
Budapest 1117
Hungary
+36 1-3722500 ext. 1202
szabados@chem.elte.hu

Peter G. Szalay
Eötvös Loránd University
Pázmány Péter Sétány 1/A
Budapest H-1117
Hungary
+36 20-5928266
szalay@chem.elte.hu

Yu Takano
Osaka University
3-2yamadaoka
Suita Osaka 5650871
Japan
+81 6-68794311
+81 6-68798636
ytakano@protein.osaka-u.ac.jp

Masako Takasu
Tokyo University of Pharmacy and Life Sciences
1432-1, Horinouchi
Hachioji
Hachioji Tokyo 192-0392
Japan
+81 42-6768918
+81 42-6768918
takasu@jc4.so-net.ne.jp



PARTICIPANTS



Teresa Tamayo-Mendoza
Universidad de Guadalajara
Loma Sombreada 8277
Loma Dorada
Tonala 45402
Mexico
33 36812657
ttamayo90@gmail.com

Samuel B. Trickey
Prof. (Emeritus)
University of Florida
QTP and Dept . of Physics
Box 118435, Univ. Florida
Gainesville FL 32611
United States
(352) 392-6978
(352) 392-8722
trickey@qtp.ufl.edu

Jules Tshishimbi Muya
Postdoctoral Researcher
University of Richmond
Grove Ave. 3524 # 6
Richmond VA 23221
United States
(804) 617-6593
julescmuya@yahoo.fr

Dayton Jonathan Vogel
University of South Dakota
5000 S. Mac Arthur Ln. #301
Sioux Falls SD 57108
United States
dytnvgl@gmail.com

Steven E. Wheeler
Assistant Professor
Texas A&M University
Department of Chemistry
PO Box 30012
College Station TX 77843
United States
(979) 862-3241
wheeler@chem.tamu.edu

Alejandro Toro-Labbé
Professor
Pontificia Universidad Católica de Chile
Av. Vicuña Mackenna 4860 Macul
Santiago
Chile
56 2-23544746
atola@uc.cl

Jonathan Trinastic
Graduate Student
University of Florida
510 SW 34th St.
22
Gainesville FL 32607
United States
(414) 331-5338
jptrinastic@phys.ufl.edu

Nicolas M. Vinson
Research Assistant
University of Florida
4000 SW 37th Blvd.
1224
Gainesville FL 32608
United States
(321) 438-0739
nmvinson@gmail.com

Yun-Peng Wang
Dr.
University of Florida
Room 2337, 2001 Museum Rd.
Gainesville FL 32611
United States
(352) 283-0446
ypwang@ufl.edu

Brian G. Wilson
Staff Physicist
Lawrence Livermore National Laboratory
7000 E. Ave.
Mail Stop L-473
Livermore CA 94550-9234
United States
(925) 423-4636
wilson9@llnl.gov



PARTICIPANTS



Chia-Hua Wu
Graduate Student
University of Georgia
1287 Cedar Shoal Dr.
517
Athens GA 30605
United States
(706) 202-6423
wujawa@uga.edu

Junchao Xia
Graduate Student
Princeton University
D314 Equad
Princeton University
Olden St.
Princeton NJ 08544
United States
(609) 258-2651
jxia@princeton.edu

Tomonori Yamada
University of Illinois
1014 E. Kerr Ave. Apt108
Urbana IL 61802
United States
(217) 402-4253
(509) 372-7133
tyamada@illinois.edu

Kizashi Yamaguchi
Professor
Osaka University
Machikaneyama 1-1
Toyonaka Osaka 560-8531
Japan
+81 6-6850 ext. 5405
+81 6-6850 ext. 5405
yama@chem.sci.osaka-u.ac.jp

Daisuke Yamaki
Research Organization for Information Science and
Technology (RIST)
Kobe KIMEC Center Building 5F
1-5-2, Minatojima-Minami-Machi, Chuo-Ku
Kobe-Shi Hyogo-Ken 650-0047
Japan
+81 78-5999562
yamaki@rist.or.jp

Shusuke Yamanaka
Associate Professor
Osaka University
Machikaneyama 1-1
Toyonaka Osaka 5600043
Japan
syama@chem.sci.osaka-u.ac.jp

Ge Yao
University of South Dakota
110 Forest Ave. # 301
Vermillion SD 57069
United States
(605) 660-2503
hugo.yao@usd.edu

David R. Yarkony
Professor
Johns Hopkins University
Department of Chemistry
3400 N. Charles St.
Baltimore MD 21212
United States
(410) 516-4663
(410) 516-8420
yarkony@jhu.edu

Chun Zhang
Assistant Professor
National University of Singapore
2 Science Dr. 3
Singapore
Singapore
phyzc@nus.edu.sg

Xiaoguang Zhang
Oak Ridge National Laboratory
111 Amanda Pl.
Oak Ridge TN 37830
United States
(865) 241-0200
xgz@ornl.gov



PARTICIPANTS



Yuchi Zhang
University of South Dakota
734 N. University St. # 317
Vermillion SD 57069
United States
(605) 670-0415
moonlzy@hotmail.com