

360° -View of Quantum Theory and Ab Initio Simulation at Extreme Conditions  
2014 Sanibel Symposium  
February 16-21, 2014

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Principal investigator: Dr. Hai-Ping Cheng

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The Sanibel Symposium 2014 was held February 16-21 2014 at the King and Prince, St. Simons Island, GA. It was successful in bringing condensed-matter physicists and quantum chemists together productively to drive the emergence of those specialties. The Symposium had a significant role in preparing a whole generation of quantum theorists. The 54<sup>th</sup> Sanibel meeting looked to the future in two ways. We had 360°-View sessions to honor the exceptional contributions of Rodney Bartlett (70), Bill Butler (70), Yngve Öhrn (80), Fritz Schaefer (70), and Malcolm Stocks (70). The work of these five has greatly impacted several generations of quantum chemists and condensed matter physicists. The “360°” is the sum of their ages. More significantly, it symbolizes a panoramic view of critical developments and accomplishments in theoretical and computational chemistry and physics oriented toward the future. Thus, two of the eight 360°-View sessions focused specifically on younger scientists. The 360°-View program was the major component of the 2014 Sanibel meeting. Another four sessions included a sub-symposium on *ab initio* Simulations at Extreme Conditions, with focus on getting past the barriers of present-day Born-Oppenheimer molecular dynamics by advances in finite-temperature density functional theory, orbital-free DFT, and new all-numerical approaches.

The proceeding of the conference are published as *Molecular Physics* vol. 113, issue 3-4 (2015).

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

# 54<sup>th</sup> Sanibel Symposium



## HONORING:

Rod Bartlett

Bill Butler

Yngve Öhrn

Henry Schaefer III

Malcolm Stocks

## SPONSORS:

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## AWARDS:

Dell-Intel

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



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## 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
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## Wednesday, February 18

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### 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
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## Friday, February 21

Plenary 15- Bartlett	21
Plenary 16- Young Stars	22
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### Symposium Party

7:00-10:00pm- Delegal Room

*Ticket required*

## List of Participants

23

## Poster Session Schedule

Inside Back Cover



# WELCOME



Welcome to the 54<sup>th</sup> 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 54<sup>th</sup> 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 54<sup>th</sup> Sanibel Symposium, we have received support from:

U.S. Department of Energy  
Basic Energy Services

Oak Ridge National Laboratory

University of Alabama

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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.



# 54<sup>th</sup> 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"> <li>Andrew Baczewski</li> <li>Mandy Bethkenhagen</li> <li>Chris Billman</li> <li>Florent Calvayrac</li> <li>Gloria Cardenas-Jiron</li> <li>Debajit Chakraborty</li> <li>James Duffy</li> <li>Boris Galabov</li> <li>Rashid Hamdan</li> <li>Yulun Han</li> <li>Thomas Jagau</li> <li>Dmitri Kiliin</li> <li>Svetlana Kilina</li> <li>Shubin Liu</li> <li>Eyal Segev</li> <li>Masako Takasu</li> <li>Jonathan Trinastic</li> <li>Nicolas Vinson</li> <li>Yun-Peng Wang</li> <li>Tomonori Yamada</li> <li>Long Zhang</li> </ol>	<ol style="list-style-type: none"> <li>Yusuke Asari</li> <li>Antonio Cancio</li> <li>Iek-Heng Chu</li> <li>Tania Cordova-Sinjiago</li> <li>Alfredo Correa</li> <li>Marta Dudek</li> <li>Tomoyuki Hamada</li> <li>Yulun Han</li> <li>Shuping Huang</li> <li>Benjamin Janesko</li> <li>Stephanie Jensen</li> <li>Xiangguo Li</li> <li>Sahar Mirshamsi</li> <li>Jeffery Mottishaw</li> <li>Monika Musial</li> <li>Wendi Sapp &amp; Adam Erck</li> <li>Paul Seybold</li> <li>Juliusz Stasiewicz</li> <li>Yu Takano</li> <li>Dayton Jonathan Vogel</li> <li>Chia-Hua Wu</li> <li>Ge Yao</li> </ol>	<ol style="list-style-type: none"> <li>Atanu Acharya</li> <li>Arie Aizman</li> <li>Hirozuki Ando</li> <li>Naveen Dandu</li> <li>Xintian Feng</li> <li>Matthew Hermes</li> <li>Youqi Ke</li> <li>Dmitry Lyakh</li> <li>Jane Murray</li> <li>Ryota Nakamura</li> <li>Akisumi Okamoto</li> <li>Ajith Perera</li> <li>Frank Pickard</li> <li>Austin Privett</li> <li>Hiroaki Saito</li> <li>Akbar Salam</li> <li>Richard Squire</li> <li>Teresa Tamayo-Mendoza</li> <li>Steven Wheeler</li> <li>Junchao Xia</li> <li>Daisuke Yamaki</li> <li>Shusuke Yamanaka</li> <li>Takehiro Yonehara</li> <li>Yuchi Zhang</li> </ol>	<ol style="list-style-type: none"> <li>Alexandre Bazanté</li> <li>Denis Bokhan</li> <li>Peter Langhoff</li> <li>Svetlana Malinovskaya</li> <li>Vladimir Malinovsky</li> <li>Jozef Noga</li> <li>Marie V. Parkes</li> <li>James J. Shepherd</li> <li>Tamar Stein</li> <li>Brian Wilson</li> </ol>	<ol style="list-style-type: none"> <li>Jason Byrd</li> <li>Tania Cordova-Sinjiago</li> <li>Tania Cordova-Sinjiago</li> <li>Mohammad H. Hasan</li> <li>Robert H. Hembree</li> <li>John Mintmire</li> <li>Takeshi Miyakawa</li> <li>Jose Juan Peña</li> <li>Scott Rabidoux</li> <li>Jules Tshishimbi Muya</li> <li>Kizashi Yamaguchi</li> </ol>



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