



The Golden Symposium of the Lise Meitner-Minerva Center Marking 20 Years of Activity

Sunday, February 12th 2017

Los Angeles Building Seminar Room, The Hebrew University of Jerusalem

Scientific Program

- 9:00-9:30 Gathering – welcome and drinks
9:30-9:55 Opening Remarks
Sason Shaik Director of the Lise-Meitner-Minerva Center, The Hebrew University of Jerusalem, Israel
"The Lise Meitner-Minerva Center - What a Marvelous Achievement It Was!"

Early Morning Session

- Chairman: **Walter Thiel**, Max Planck Institute Mülheim, Germany
9:55 – 10:20 **Martin Kaupp**, Technische Universität Berlin, Germany
"Recent Progress on Local Hybrid Functionals"
10:20 – 10:45 **Jürgen Gauss**, Johannes Gutenberg Universität Mainz, Germany
"Equation-of-Motion Coupled-Cluster Theory for Ionized States: a Versatile Tool for the Treatment of Open-Shell Systems"
10:45 – 11:10 **Frank Neese**, MPI für Chemische Energiekonversion, Mülheim, Germany
"Coupled Cluster Theory for Systems with Hundreds of Atoms: Progress and Perspectives"
11:10 – 11:25 **Inbal Oz**, Tel Aviv University, Israel
"Simulating Non-Equilibrium Thermodynamics in Open Quantum Systems"
11:25 – 11:50 COFFEE BREAK

Late Morning Session

- Chairman: **Roy Shenhar**, The Hebrew University of Jerusalem, Israel
11:50 – 12:15 **Sason Shaik**, The Hebrew University of Jerusalem, Israel
"One's Personal Account on Science During the Membership in the Lise Meitner Center".
12:15 – 12:40 **Johannes Kaestner**, Universität Stuttgart, Germany
"Atom Tunneling as a General Phenomenon in Chemistry: from the Interstellar Medium to Enzymes"
12:40 – 13:05 **Johannes Neugebauer**, Wilhelms Universität Münster, Germany
"Advanced QM/QM-Embedding Methods"
13:05 – 13:20 **Anil R. Mhashal**, Bar-Ilan University, Israel
"Effect of Asp122 Mutations on E. Coli DHFR: Structure and Dynamics"

13:20 – 14:30 LUNCH + POSTER SESSION

Early Afternoon Session

- Chairman: **Ilan Marek**, Technion-Israel Institute of Technology
- 14:30 – 14:55 **Stefan Grimme**, Universität Bonn, Germany
"Calculation of Electron Ionization Mass Spectra by Quantum Chemistry"
- 14:55 – 15:20 **Andreas Dreuw**, Ruprecht-Karls Universität Heidelberg, Germany
"Organic Photochemistry Using ADC-Based Methods"
- 15:20 – 15:45 **Robert Berger**, Philipps Universität Marburg, Germany
"Light and Cool Molecules – Theory for Laser Cooling of Polyatomic Systems"
- 15:45 – 16:00 **Soumyajit Sarkar**, Weizmann Institute of Science, Israel
"First Principles Theory of Selected Collective Effects at the Metal/Molecule Interface"
- 16:00 – 16:25 **Ori Gidron**, The Hebrew University of Jerusalem, Israel
Michael Bendikov Memorial Lecture
"The Chemistry of Oligofurans: Recent Advances and Future Prospects"
- 16:25 – 16:50 COFFEE BREAK

Late Afternoon Session

- Chairman: **David Milstein**, Weizmann Institute of Science, Israel
- 16:50 – 17:15 **Markus Reiher**, ETH Zürich, Germany
"Interactive and Automated Exploration of Reaction Mechanisms"
- 17:15 – 17:40 **Hendrik Zipse**, Ludwig-Maximilians-Universität München, Germany
"The Silylation of Alcohols"
- 17:40 – 18:05 **Yitzhak Apeloig**, Technion-Israel Institute of Technology
"Scaling Computationally the π -Acceptor and σ -Donor Properties of Cyclic Aminocarbenes"
- 18:05 – 18:20 Closing Remarks
Helmut Schwarz, Chair of the Beirat, Technische Universität Berlin, Germany

Registration Site: <https://indico.phys.huji.ac.il/indico/event/3/> (free)