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**Bartlett Lecture**Session Chairman: **David Magers**  
*Mississippi College***Rodney J. Bartlett**  
*University of Florida*

Coupled-Cluster Theory in Quantum Chemistry: The Emergence of a New Paradigm

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**2<sup>nd</sup> Session**Session Chairman: **Paul B. Tchounwou**  
*Jackson State University***Alexander D. MacKerell, Jr**  
*University of Maryland*

Development of a Polarizable Force Field Based on the Classical Drude Oscillator

**Darrin M. York**  
*University of Minnesota*

Molecular Simulation and Quantum Chemical Studies of Ribozyme Catalysis

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**3<sup>rd</sup> Session**Session Chairman: **Charles R. Welch**  
*US Army ERDC***Yasuyuki Ishikawa**  
*University of Puerto Rico*

A Combined Direct Molecular Dynamics/Density-Functional Theoretical Study of the Electrochemical Hydrogen Oxidation Reaction and Underpotential Deposition of H on Pt(111)

**Kwang S. Kim**  
*Pohang University of Science and Technology*

Magic Structures and Quantum Conductance of Linear Ultrathin Nanowires and Negative Differential Resistance of Molecular Wires

**Szczepan Roszak**  
*Wroclaw University of Technology*

The bonding and structural and thermodynamic properties of metal-carbon and metal-silicon compounds – building blocks of same nanomaterials

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**4<sup>th</sup> Session**Session Chairman: **Jaroslav Burda**  
*Charles University***Sharon Hammes-Schiffer**  
*Pennsylvania State University*

Nuclear-Electronic Orbital Approach: Including Nuclear Quantum Effects in Electronic Structure Calculations

**Manthos G. Papadopoulos**  
*National Hellenic Research Foundation*

The Linear and Nonlinear Optical Properties of a Series of Derivatives Involving One or More Noble Gas Atoms

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**5<sup>th</sup> Session**Session Chairman: **Hongtao Yu**  
*Jackson State University***Thomas C. Schulthess**  
*Oak Ridge National Laboratory*

Self-Interaction Corrected Local Spin Density Calculations in Strongly Correlated Electron Materials

**Takahito Nakajima**  
*University of Tokyo*

Large-Scale Molecular Theory

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**6<sup>th</sup> Session**Session Chairman: **Fillmore Freeman**  
*University of California, Irvine***Vincent Ortiz**  
*Auburn University*

Three Approaches to a Nonlocal, Energy-Dependent Correlation Potential in Electron Propagator Theory

**Roberto Cammi**  
*Universita' di Parma*

Structure and Properties of Molecular Solutes in Electronic Excited States: a Polarizable Continuum Model Approach Based on the Time Dependent Density Functional Theory