

# 40<sup>TH</sup> MIDWEST THEORETICAL CHEMISTRY CONFERENCE PROGRAM

JUNE 26–JUNE 28, 2008  
930 NORTH UNIVERSITY AVE  
CHEMISTRY BLDG  
LECTURE HALL #1640

## THURSDAY, JUNE 26TH

- 5:00-9:00 pm**      **Registration and check-in** (Chemistry Building Atrium)
- 6:00-9:00 pm**      **Opening Reception & pizza dinner** (Chemistry Building Atrium)
- 7:30-9:00 pm**      **Poster Session I & refreshments** (Chemistry Building Atrium)

## FRIDAY, JUNE 27TH

- 7:00-8:20 am**      **FULL BREAKFAST** (Chemistry Building Atrium)
- 8:20-8:30 am      Eitan Geva & Barry Dunietz (University of Michigan – Conference Organizers)  
*Opening Remarks*
- 8:30 am-12:00pm      *Morning session; Presiding: Barry Dunietz (University of Michigan)*
- 8:30-9:10 am      Krishnan Raghavachari (Indiana University)  
*“QM/QM Electronic Embedding Models for Materials Chemistry”*
- 9:10-9:30 am      Trilisa M. Perrine (University of Michigan)  
*“Molecular Conductance: Single Molecule Switches”*
- 9:30-9:50 am      Gergely Gidofalvi (Argonne National Laboratory)  
*“Electronic Structure Calculations with Nonlinear Basis Expansions”*
- 9:50-10:10 am      Isaiah Sumner (Indiana University)  
*“Incorporating Nuclear Quantum Effects in the Dynamics of Large Systems Through Quantum Wavepacket ab initio Molecular Dynamics and QM/MM Techniques”*
- 10:10-10:40 am**      **COFFEE BREAK & SNACKS (Chemistry 1<sup>st</sup> floor Atrium)**
- 10:40-11:00 am      Berit Mannfors (University of Michigan)  
*“Physically Enhanced Treatment of Hydrogen Bonding in Molecular Mechanics Energy Functions: The SDFW Water Dimer”*
- 11:00-11:20 am      Mingli Xiang (Western Michigan University)  
*“Effect of Resonance on Inter- and Intra-Molecular Hydrogen bond: A Study with Block-localized Wave function (BLW) Method”*

- 11:20-11:40 am Eugene DePrince (University of Chicago)  
*"The Parametric Approach to Variational 2-RDM Methods"*
- 11:40-12:00 pm Carolyn Phillips (University of Michigan)  
*"Effects of Nanoparticle Size Polydispersity on Stability of the Double Gyroid Phase in a Tethered Nanoparticle System"*
- 12:00-1:30 pm LUNCH (on your own)**
- 1:30-5:00 pm *Afternoon session; Presiding: E. Geva (University of Michigan)*
- 1:30-2:10 pm Shaul Mukamel (University of California Irvine)  
*"Quasiparticle description of Coherent Multidimensional Optical Spectroscopy of Excitons; Life on the Schwinger Loop"*
- 2:10-2:30 pm Gabriel Hanna (University of Michigan)  
*"A Computational Study of the 1D and 2D Infrared Spectra of a Vibrational Mode Strongly Coupled to its Environment"*
- 2:30-2:50 pm Irina Navrotskaya (Pennsylvania State University)  
*"Nonadiabatic Rate Constants for Electrochemical Proton-Coupled Electron Transfer Based on a Model System-bath Hamiltonian"*
- 2:50-3:10 pm Sara E. Ray (Ohio State University)  
*"Determining the Role of Vibrational Excitation on the Dynamics of the Hydrogen Transfer Reaction of F(2P)+HCl → FH + CL(2P)"*
- 3:10-3:40 pm COFFEE BREAK & SNACKS (Chemistry 1<sup>st</sup> floor Atrium)**
- 3:40-4:00 pm Porscha L. McRobbie (University of Michigan)  
*"Theory and Simulation of Multidimensional Nonlinear Spectroscopy"*
- 4:00-4:20 pm Matthew Kundrat (SUNY at Buffalo)  
*"Modeling the Effects of an Achiral Solvent on the Chiroptical Response of Chiral Amino Acids"*
- \*NEW SPEAKER FOR 4:20pm SLOT\***
- 4:20-4:40 pm Alexander Prociuk (University of Michigan)  
*"Time-dependent NEGF Calculations of Extended Systems"*
- 4:40-5:00 pm Xiaohu Li (Indiana University)  
*"Key Insights on "temperature-dependent" Gas-phase Vibrational Spectroscopy: Case Study of the Hydroxide Water Cluster and the Proton Bound Dimethyl Ether Dimer"*
- 5:00-7:00 pm Poster Session II & refreshments (Chemistry Building Atrium)**
- 7:30-10:00 pm BANQUET (BALLROOM IN THE MICHIGAN UNION)**

## SATURDAY, JUNE 28TH

- 7:00-8:30 am**      **FULL BREAKFAST (Chemistry Building Atrium)**
- 8:30 am-12:00pm    *Morning session; Presiding: Charles L. Brooks III (University of Michigan)*
- 8:30-9:10 am      Christopher J. Cramer (University of Minnesota)  
*“Electronic Structure Challenges Associated with Dioxygen Activation at Mono and Binuclear Copper Enzyme Site Models”*
- 9:10-9:30 am      Jason L. Sonnenberg (Wayne State University)  
*“The Search for a Double-Stuffed Uranium Metallocene”*
- 9:30-9:50 am      Mary Rohrdanz (Ohio State University)  
*“Simultaneous Benchmarking of Ground- and Excited-state Properties with Long-Range-Corrected Density Functional Theory”*
- 9:50-10:10 am     Amir Karton (Weizmann Institute of Sciences)  
*“W4 Theory for Computational Thermochemistry: in Pursuit of Confident Sub-kJ/mol Predictions”*
- 10:10-10:40 am**    **COFFEE BREAK & SNACKS (Chemistry Building Atrium)**
- 10:40-11:20 am    Carol Post (Purdue University)  
*“Hints from Compressibility on the Role of Buried Charge on Protein Structural Stability”*
- 11:20-11:40 am    Ron Hills (The Scripps Research Institute)  
*“Coevolution of Function and the Folding Landscape”*
- 11:40-12:00 pm    Peng Tao (Wayne State University)  
*“Matrix Metalloproteinases 2 (MMP2) Inhibition: DFT and QM/MM Studies of the Inhibition Mechanism of SB-3CT and its Analogs”*
- 12:00-12:20 pm    Guowei Wei (Michigan State University)  
*“Formation and Evolution of Biomolecular Surfaces”*
- 12:20-12:30 pm**    **Concluding Remarks**  
Eitan Geva & Barry Dunietz (University of Michigan)