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  COFFEE BREAK & SNACKS (Chemistry 1st floor Atrium)

10:10-10:40 am  COFFEE BREAK & SNACKS (Chemistry 1st floor Atrium)

10:40-11:00 am  Berit Mannfors (University of Michigan)
“Physically Enhanced Treatment of Hydrogen Bonding in Molecular Mechanics Energy Functions: The SDFF 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 Æ FH + CL(2P)”

3:10-3:40 pm  COFFEE BREAK & SNACKS (Chemistry 1st 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-12:00 pm  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)