Friday, November 10, 2017

8:00A – 12:00P	Registration	
8:00A – 9:00A	Coffee and morning snacks	
9:00A – 9:10A	Opening Remarks	
9:10A – 10:10A	**1st Session** *Session Chair: Gregory Tschumper*	**Svein Saebo**: "Overview of Peter Pulay's Career and Accomplishments" **Peter Pulay**: "Strong Electron Correlation: The Last Frontier"
10:10A – 10:30A		*Coffee Break / Pictures*
10:30A – 12:00P	**2nd Session** *Session Chair: Agnieszka Gajewicz*	**Anna Krylov:** "Electronic Resonances: Challenge and Opportunity" **George Schatz:** "SERS, TERS and Plasmon-Enhanced Energy Transfer" **Kenneth Jordan:** "Treating Electron Correlation Effects Using One-Electron Model Hamiltonians"
12:00P – 1:30P	Lunch	
1:30P – 3:00P	**3rd Session** *Session Chair: Fillmore Freeman*	**Kwan-Soo Kim:** "Interplay Between Theory & Experiment Towards Novel Optics/Electronics/Spintronics and Efficient Energy Conversion" **Stefan Grimme:** "Applications of the Extended Tight Binding Method (GFN-xTB)" **Vincent Ortiz:** "Correlation-Bound Anions and Their Dyson Orbitals"
3:00P – 4:30P	**4th Session** *Session Chair: Jane Murray*	**Joan-Emma Shea:** "Effect of Surfaces and Osmolytes in Modulating Peptide Assembly" **Mattanjah de Vries:** "How Nature Covers Its Bases: Interplay Between Theory and Experiment" **Janusz Rak:** "Photoexcited Electron Transfer in Double-Stranded DNA Labelled with 5-Bromo-2'-Deoxyuridine. Marcus Theory Calculations and Damage Measurements Employing High Resolution Mass Spectrometry"
4:30P – 5:00P	Coffee Break	
5:00P – 6:30P	**1st Poster Session (P1)**	
6:30P – 8:30P	Dinner	

Saturday, November 11, 2017

8:00A – 9:00A	Coffee and morning snacks	
8:30A – 11:00A	Registration	
9:00A – 10:30A	**5th Session** *Session Chair: Andrzej Wierzbicki*	**Ewa Broclawik:** "Spin Status and Zeolitic Environment as Factors Controlling Electron Density Transfer for Co(II)-NO Adducts in Zeolites: WF, DFT and Periodic Modeling" **Attila Csaszar:** "Molecules in Motion" **William Lester:** "Quantum Monte Carlo for Molecular Systems: Electronic Structure"
10:30A – 11:00A	Coffee Break	
11:00A – 12:30P	**6th Session** *Session Chair: Tomasz Puzyn*	**Daniel T. Crawford:** "Streamlining Coupled Cluster Response Theory" **John Stanton:** "Active Thermochemical Tables: What It Is, Why I Care About It, and Why You Should, Too" **Krzysztof Szalewicz:** "Do Semilocal Density-Functional Approximations Partly Recover Dispersion Energies Near van der Waals Minima?"
12:30P – 2:00P	Lunch	
2:00P – 3:30P	**7th Session** *Chairperson: Damien Riedel*	**Peter Knowles:** "Single-Reference Electron Correlation Methods for Multireference Problems" **Shuhua Li:** "New Electronic Structure Methods for Strongly Correlated Systems" **Filipp Furche:** "Variational Generalized Kohn-Sham Approach Combining Random Phase Approximation and Green's Function Methods"
3:30P – 4:00P	Coffee Break	
4:00P – 5:30P	**2nd Poster Session (P2)**	
6:00P – 9:00P	Conference Banquet Speaker Introduction of speaker: **Dr. Cary Chabalowski**	"Gradients of Computational Chemistry: From Current Trends to Future Opportunities" **Dr. Angela Wilson,** *John A. Hannah Distinguished Professor* Department of Chemistry Michigan State University