Friday, November 9, 2018

8:00A – 12:00P	Registration	
8:00A – 9:00A	Coffee and morning snacks	
9:00A - 9:10A	Opening Remarks	
9:10A - 10:40A	**1st Session** **Session Chair: TBA**	**Prof. Henry F. Schaefer** "Quantum Chemistry and Large Scale Computations: A Tightly Coupled Parallel Development" **Richard Wong Ming Wah** "Applications of Halogen Bonding to Supramolecular Chemistry, Phosphorescence Materials and Catalysis"
10:40A–11:00A	Coffee Break / Pictures	
11:00A–12:30P	**2nd Session** **Session Chair: TBA**	**Leslie Vogt-Maranto** **"**Molecular dynamics via machine learning: Predicting energies from electron densities" **Masataka Nagaoka** **"**Red Moon Methodology: A Computational Molecular Technology for Complex Chemical Reaction Systems - Its Theoretical Treatment and Applications"
12:30P -2:00P	Lunch	
2:00P -3:30P	**3rd Session** **Session Chair: TBA**	**Marivi Fernández-Serra** **"**Evaluating photocatalytic active sites as function of polarization, level alignment and spontaneous dissociation of hydroxyl groups at perovskite oxide surfaces" **Laura Gagliardi** **"**Computationally Guided Discovery of Metal–Organic Frameworks Active for Catalysis"
3:30P -3:50P	Coffee Break	
3:50P – 5:30P	First Poster Session (P1)	
6:00P – 8:00P	Dinner	

Saturday, November 10, 2018

8:00A – 9:00A	Coffee and morning snacks	
8:30A – 11:00A	Registration	
9:00A – 10:30A	**4th Session** **Session Chair: TBA**	**Margarita Isabel Bernal Uruchurtu "**A tale of water and halogens and the toolbox needed to unveil their narrative" **Tomasz Puzyn "**Towards computational risk assessment of ionic liquids"
10:30A -10:50A	Coffee Break	
10:50A-12:20P	**5th Session** **Session Chair: TBA**	**Katharina Boguslawski "**Inexpensive wave-function-based methods to model ground and excited states in challenging systems" **Frank Hagelberg "**Zigzag Nanoribbons as Media for Spin Transmission"
12:20P – 2:00P	Lunch	
2:00P – 4:15P	**6th Session** **Session Chair: TBA**	**YounJoon Jung "**Computer Simulation Study of Differential Capacitance and Charging Mechanism in Ionic Liquid-Based Graphene Supercapacitors" **Jozef Adam Liwo "**Physics-based scale- and geometry-consistent coarse-grained potentials" **Joachim Sauer "**Ab initio calculations with chemical accuracy for molecule - surface interactions and the performance of DFT+dispersion"
4:15P- 4:40P	Coffee Break	
4:40P- 6:00P	**2nd Poster Session** (P2)	
6:30P – 9:00P	Banquet	Banquet Speaker **David Horner**, Director of ERDC ITL