

Friday, November 8, 2019

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: P. Pulay	Rodney Bartlett “The Devil’s Triangle In KS-DFT Calculations And How To Fix It” Donald Truhlar “Recent Progress in Kohn-Sham Density Functional Theory and Multi-Configuration Pair-Density Functional Theory”
10:40A–11:20A	Coffee Break / Pictures	
11:20A–12:50P	2nd Session Session Chair: F. Freeman	Adriana Pietropaolo “Towards a bespoke design of chiral photoswitches operating away from the global free-energy minimum” Jared Delcamp “Small Molecule NIR Dye Design and Understanding Made Possible with Computational Chemistry”
12:50P -2:20P	Lunch	
2:20P -3:50P	3rd Session Session Chair: H. Yu	Adam Willard “The statistical mechanics of hydrogen bonding at the liquid water interface” Dean Tantillo “Post-transition State Dynamics for Organic Reactions”
3:50P -4:20P	Coffee Break	
4:20P – 6:00P	First Poster Session (P1) Chair: B. Rasulev	
6:00P – 8:00P	Dinner	Dinner Speaker - Davita Watkins

Saturday, November 9, 2019

8:00A – 9:00A	Coffee and morning snacks	
8:30A – 11:00A	Registration	
9:00A – 10:30A	4th Session Session Chair: A. Sygula	Roberto Car “Boosting ab-initio molecular dynamics with machine learning” Adama Tandia “Artificial Intelligence for glass composition design: advances and remaining challenges”
10:30A -10:50A	Coffee Break	
10:50A-12:20P	5th Session Session Chair: A. Wierzbicki	Jane Murray “Polarization in Noncovalent Interactions” Liudmil Antonov “Tautomerism: theory and experiment playing together”
12:20P – 2:00P	Lunch	
2:00P – 4:15P	6th Session Session Chair: M. Shukla	Alicia Mikolajczyk “Lessons from the past, vision for the future: Application of Nano-QSAR for design of safe nanomaterials” Minh Tho Nguyen “The Quasi-planar Boron Clusters: Formation, Topology and Aromaticity” Igor Alabugin “Computational Analysis of Electronic Effects on Structure and Reactivity: From Hybridization to Stereoelectronics to Electron Upconversion”
4:15P- 4:30P	Coffee Break	
4:30P- 6:00P	Second Poster Session (P2) Chair: D. Magers	
6:00P – 9:00P	Banquet	Banquet Speaker - Robert Wallace