ACS Award for Research at an Undergraduate Institution: Symposium in Honor of George C Shields

ACS Division of COMP Computers in Chemistry

Mile High Ballroom 1E • Colorado Convention Center

Monday, March 23, 2015 (Afternoon)

1:30	Introductory Remarks
1:40	Christopher J Cramer *Concertedness and synchronicity—from arynes to electrochemistry*
2:10	Thomas E Morrell *Molecular simulations in conjunction with experimental studies illustrate internal protein logic controlled by conformation and dynamic structural change*
2:30	Katrina W Lexa *Predicting permeability and target binding of complex macrocycles*
3:00	Intermission
3:20	Carol A Parish *Molecular studies of halogen bonding, protein folding and combustion*
3:50	Kaye A Archer *Anharmonic effects in vibrational spectra of protonated water clusters*
4:10	Matthew D Liptak *Insight into hydrazone-based dye fluorescence from density functional theory*
4:40	Frank C Pickard *Recent developments in high accuracy non-bonded interactions in the CHARMM simulation package*
5:10	Kelly E Anderson *Examining the interface: simulations exploring the effect of solid substrates on thin liquid films*

Tuesday, March 24, 2015 (Morning)

8:30	Kenneth M Merz *Thermodynamic quantities and structural information from a molecular printing press*
9:00	Katherine Alser *Addressing problems at the interface of chemistry and medicine: computational and chemical biology approaches*
9:20	Marco A Allodi *From the atmosphere to the interstellar medium: long-range molecular interactions*
9:40	Intermission
10:00	Kenneth D Jordan *Comparison of diffusion Monte Carlo and CCSD(T) methods on model systems*
10:30	Karilyn Larkin *From the computational chemistry lab to treating cancer: inspiration for drug development in our time*
10:50	Berhane Temelso *Evolution of methods for modeling hydrogen-bonded systems accurately and efficiently*
11:20	Maria C Nagan *Role of water in arginine-rich motif peptide-RNA recognition*

Tuesday, March 24, 2015 (Afternoon)

1:30	Adrian E Roitberg *On things that move. Protons, electrons, and other beasts in molecular modeling*
2:00	Heather Brummel McCuen *Highlights of a science career that began with undergraduate research*
2:20	Edward C Sherer *Computational chemistry's impact beyond discovery chemistry: spectroscopy, cheminformatics and application of density functional theory in support of process/analytical chemistry*
2:50	Intermission
3:10	Karl Kirschner *It's all about the fundamentals*
3:40	Scott Feller *Conformation of retinal controls the pKa of protonated Schiff base during rhodopsin activation*
4:10	Marcus Jurema *Role of quantum chemistry, PM3 and magic water clusters in unlocking Rodin's "Gates of Hell"*
4:30	George C Shields *Research with undergraduates - a fabulous career*

Organizers: Edward C Sherer & George C Shields

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