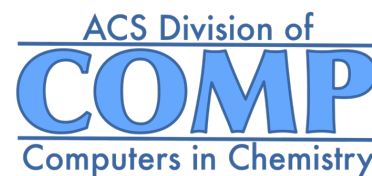


ACS Award for Research at an Undergraduate Institution: Symposium in Honor of George C Shields



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*