

# SETCA

2009 ANNUAL MEETING OF SOUTHEASTERN THEORETICAL CHEMISTRY ASSOCIATION



Duke University

Room 2231 - French Family Science Center

May 15-16, 2009

Sponsored by:

**Silicon Graphics**



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**Fitzpatrick Institute for Photonics (FIP)**



**Mathematica**



**Dr. Micah Abrams**

Organized by:

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Special thanks to Cecilia Eichenberger and Dr. Xiangqian Hu for assistance.

## Friday (May 15, 2009)

- 8:30 am Registration  
**Session Chair: Paula Mori-Sánchez**, Duke University
- 9:00 am [Akbar Salam](#), Wake Forest University  
*Long-range intermolecular interactions via the method of induced moments*
- 9:30 am [Steven Wheeler](#), University of Georgia  
*Through-space effects of substituents on non-covalent interactions and molecular electrostatic potentials of Arenes*
- 9:45 am [Vitaly Rassolov](#), University of South Carolina  
*Semi-classical electron correlation operator*
- 10:15 am [Xiangqian Hu](#), Duke University  
*A gradient-directed Monte Carlo approach to molecular design*
- 10:30 am Break  
**Session Chair: Micah Abrams**, Decisive Analytics Corporation
- 10:50 am [Hao Hu](#), Hong Kong University  
*Catalysis and conformational dynamics of well structured wild-type and molten globular mutant chorismate mutases*
- 11:20 am [Kyungwha Park](#), Virginia Tech  
*Electron transport through the single-molecule magnet  $Mn_{12}$*
- 11:35 am [Shengli Zou](#), University of Central Florida  
*Raman scattering enhancement and fluorescence quenching around a metal nanoparticle*
- 12:05 am [Erin Johnson](#), Duke University  
*Implications of delocalization error for thermochemistry and bonding*
- 12:20 am Lunch (French Family Science Center)  
**Session Chair: Joseph Buchanan**, Silicon Graphics
- 1:40 pm [Garegin A. Papoian](#), The University of North Carolina at Chapel Hill  
*Atomistic and coarse-grained modeling of DNA and chromatin*
- 2:10 pm [Yongmei Wang](#), University of Memphis  
*Multiscale modeling of DNA condensation by polycations*
- 2:25 pm [Bin Chen](#), Louisiana State University  
*Towards understanding the nucleation mechanism for multi-component systems: an atomistic approach*
- 2:55 pm [Yaroslava Yingling](#), North Carolina State University  
*Understanding self-assembly of nucleic acids into advanced materials*
- 3:10 pm Break  
**Session Chair: William A. Glauser**, Schrödinger Inc.
- 3:30 pm [Carlen Ben](#), The University of Tennessee - Knoxville  
*X-ray absorption spectra within the core-hole approximation: an implementation in NWChem*

- 3:45 pm [Michael-Rock Goldsmith](#), US-Environmental Protection Agency  
*Prenatal plasma proteins, Playstation 3 and predictive models for public health: a-fetoprotein alliterated*
- 4:00 pm [Yi-Qin Gao](#), Texas A&M University  
*The hydrophobic and hydrogen bonding interactions in polypeptides*
- 4:30 pm [Ram Prasad Bora](#), University of Miami  
*Enzyme-substrate ( $A\beta 40$  and  $A\beta 42$ ) interactions and the catalytic mechanism of insulin degrading enzyme (IDE)*
- 4:45 pm [Brian Dominy](#), Clemson University  
*Towards a biophysical characterization of enzyme evolution*
- 5:00 pm Poster & Reception
- 7:00 pm Dinner (French Family Science Center)

### Saturday Morning (May 16, 2009)

- Session Chair: David Sherrill**, Georgia Institute of Technology
- 8:30 am [Edward Valeev](#), Virginia Tech  
*Recent advances in explicitly-correlated electronic structure methods*
- 9:00 am [Ilya Balabin](#), Duke University  
*Coarse-grained modeling of signal transduction in GPCRs*
- 9:15 am [Daniel Kosov](#), University of Maryland  
*Attosecond chemistry*
- 9:45 am [Gabor Czako](#), Emory University  
*Accurate ab initio potential energy surface, dynamics, and thermochemistry of the  $F + CH_4 \rightarrow HF + CH_3$  reaction*
- 10:00 am Break
- Session Chair: Shahar Keinan**, Duke University
- 10:20 am [Stefano Curtarolo](#), Duke University  
*Disorder-order transitions in Fe nano-catalysts*
- 10:50 am [Wes Crill](#), North Carolina State University  
*Atomistic+continuum multi-scale modeling of single asperity gold-gold contact in an RF MEMS device*
- 11:05 am [Melissa Pasquinelli](#), North Carolina State University  
*Molecular simulations of carbon nanotubes wrapped with polymers*
- 11:20 am [Xiongce Zhao](#), Oak Ridge National Laboratory  
*Simulation study of interaction between DNA and  $C_{60}$*
- 11:50 am SETCA annual meeting

(Abstracts of talks and posters are available at:

[http://www.chem.duke.edu/2009/SETCA/abstract/SETCA\\_abstract\\_organized.pdf](http://www.chem.duke.edu/2009/SETCA/abstract/SETCA_abstract_organized.pdf).)