

# T6: Coupling Theory, Molecular Simulations and Computational Chemistry to the Physical World

**To Use this Index:** Scroll down or use the bookmarks in the left-hand frame to move to a new location in this index. Click on a [blue paper title](#) to view that paper. To return to this index after viewing a paper, click the PREVIOUS MENU bookmark in the left frame.

## Session 42 - Nanoscale Systems II: Frontiers in Nanoscience and Technology (invited talks) \*

Chair: Lev Gelb

Vice Chair: Janna K Maranas

## Session 43 - Plenary: "Coupling Theory, Molecular Simulations and Computational Chemistry to the Physical World" \*

Chair: Peter T Cummings

Vice Chair: Joe T Golab

## Session 44 - Multiscale Modeling III: Methods to Advance Length and Time-Scale Representation in Modeling

Chair: Kristen A Fichthorn

Vice Chair: Kendall T Thomson

44e [Simulating fluctuating mesoscopic dynamics using three dimensional Voronoi cells](#)  
*E.A.J.F. Peters*

## Session 45 - Computational Chemistry and Molecular Simulation I

Chair: Phillip R Westmoreland

Vice Chair: Clare McCabe

45g [PVC/LDPE incompatible blends for industrial applications: a computational multiscale approach](#)  
*M. Fermeglia, A. Coslanich, M. Ferrone, T. Humar, M.S. Paneni, S. Pricl, E. Paglione*

## Session 46 - Computational Chemistry and Molecular Simulation II

Chair: Phillip R Westmoreland

Vice Chair: Clare McCabe

46a [Steps to a Bridge: Multiscale Modeling of the Thermodynamics of a Fluid](#)  
*Steven G. Arturo and Dana E. Knox*

46c [Ultraviolet Absorbers in Polymer Studied by Molecular Simulation](#)  
*Yogesh Srivastava and Michael L. Greenfield*

46h [Solvent effects on the beta-cyclodextrin inclusion complexes with m-cresol and dynamic hydrophobicity: molecular dynamics](#)  
*Kailiang Yin, Qing Xia, Duanjun Xu*

## Session 47 - Molecular Modeling Methods I: Recent advances in Molecular Dynamics

Chair: Jonathan Moore

Vice Chair: Jeffrey R Errington

47h [Replica Exchange Molecular Dynamics Modeling of Foldamers](#)  
*Bamidele Adisa, David Bruce and Jay McAliley*

## Session 48 - Nanoscale Systems I: Water in Heterogeneous Environments

Chair: Bernhardt L Trout

Vice Chair: J. Ilja Siepmann

48a [Molecular Dynamics Simulation of Methane Hydrate Dissociation](#)  
*Niall J. English*

48e [Pressure Denaturation of Proteins in Water: Revisiting a Heteropolymer Collapse Model](#)  
*Pooja Shah, Thomas M. Truskett*

## Session 49 - Simulation of Biomolecules I: Computational Representation of Genomics and Proteomics

Chair: Grant S Heffelfinger

Vice Chair: Charles M Roth

- 49c [MicroarrayCAKE: a simulation and analysis framework to guide experimental design and gene expression data analysis](#)  
*Rajanikanth Vadigepalli, Rishi Khan, Guang Gao and James Schwaber*
- 49d [Support Vector Clustering of Microarray Data](#)  
*Ozlem Yilmaz, Luke.E.K.Achenie and Ranjan Srivastava*
- 49e [Integrative Data-Driven Mathematical Models Predict Novel Genomescale Correlation Between Dna Replication Initiation and Rna Transcription During the Cell Cycle in Yeast](#)  
*Orly Alter, Gene H. Golub, Patrick O. Brown and David Botstein*

## Session 50 - Molecular Modeling Methods II: Recent Advances in Monte Carlo methods

Chair: Jeffrey J Potoff

Vice Chair: Lev Gelb

- 50c [Biomolecular Free Energy Profiles by a Shooting/Umbrella Sampling Protocol \("BOLAS"\)](#)  
*Ravi Radhakrishnan*
- 50h [Simulating fluid-crystalline solid equilibria with the Gibbs ensemble](#)  
*M.B. Sweatman and N. Quirke*

## Session 51 - Electronic Materials II: Computational and Experimental Studies of Polymers for Microelectronics and Photonics

Chair: Peter Ludovice

Vice Chair: Lynn Loo

- 51c [Parasitic resistance in bottom-contact pentacene thin-film transistors that use water-dispersible polyaniline electrodes](#)  
*Kwang Seok Lee, Graciela B. Blanchet, Feng Gao and Yueh-Lin Loo*
- 51d [Organic solvent processable Oligotron™ conducting triblock copolymers for microelectronics: functional end-capped conducting oligomers](#)  
*Brian J. Elliott, William W. Ellis, Silvia Luebben and Shawn Sapp*
- 51e [Immersion Lithography: Moving Microlithography to Nanolithography](#)  
*J. Christopher Taylor, Charles R. Chambers, Ramzy M. Shayib, Robert J. LeSuer, Willard E. Conley and C. Grant Willson*

## Session 52 - Simulation of Biomolecules II: Computational Biology \*

Chair: Abraham D Stroock

Vice Chair: Grant S Heffelfinger

## Session 53 - Molecular Modeling Methods III: Developments in intermolecular potential models

Chair: Marcus Martin

Vice Chair: Matthew Neurock

- 53e [Transferable Step Potentials for Amines, Primary Amides, Ketones, Thiophenes, Phosphates, and Chlorinated Hydrocarbons](#)  
*Amanda Sans, F. Suhan Baskaya, Neil H. Gray, Zeynep N. Gerek and J. Richard Elliott*

## Session 54 - Simulation of Biomolecules III: Computational Biology

Chair: Vassily Hatzimanikatis

Vice Chair: Kris Chan

- 54a [DNA Synthesis Efficiency and Fidelity Mechanisms](#)  
*Ravi Radhakrishnan*

### **Session 55 - Nucleation**

Chair: Bernhardt L Trout

Vice Chair: David S Corti

- 55c            [Nucleation of Monovalent Metal Particles from Metastable Vapor](#)  
*Ranjit Bahadur and Richard B. McClurg*
- 55d            [System size dependence of the free energy surface in cluster simulation of nucleation](#)  
*Isamu Kusaka*
- 55g            [Bubble nucleation in micellar solution: A density functional study](#)  
*Pankaj A. Apte and Isamu Kusaka*

### **Session 56 - Molecular Modeling Methods IV: Simulation of Materials Processing \***

Chair: Talid R Sinno

Vice Chair: Phillip R Westmoreland

### **Session 57 - Computational Chemistry and Molecular Simulation III**

Chair: Phillip R Westmoreland

Vice Chair: Clare McCabe

- 57e            [Quantum Chemical Prediction of Hydrocarbon Cracking Reactions](#)  
*Xiaobo Zheng and Paul Blowers*

### **Session 58 - Multiscale Modeling II: Multiscale Characterization and Modeling of Polymers**

Chair: Sanat Kumar

Vice Chair: Cameron F Abrams

- 58c            [Characteristics of parameter reduction in multiscale simulations of polymer chains](#)  
*Ahmed E. Ismail, George Stephanopoulos and Gregory C. Rutledge*

### **Session 439 - Multiscale Modeling and Simulation I**

Chair: Dionisios G Vlachos

Vice Chair: Martha Gallivan

- 439a            [Simulation of Copper Nanostructure Formation by Coupling Kinetic Monte Carlo Simulation, Continuum Models, and the Level Set Method](#)  
*Timothy O. Drews, Effendi Rusli, Yuan He, Xiaohai Li, Richard C. Alkire and Richard D. Braatz*
- 439b            [Predictor-Corrector Methods for Dynamically Coupling Multiscale Simulation Codes](#)  
*Yuan He, Joshua Gray, Richard C. Alkire and Richard D. Braatz*
- 439g            [Design of an Optimal Overlap Algorithm for Dynamically Coupling Continuum and Noncontinuum Codes in Multiscale Simulation](#)  
*Effendi Rusli and Richard D. Braatz*

### **Session 441 - Multiscale Modeling and Simulation II \***

Chair: Dionisios G Vlachos

Vice Chair: Martha Gallivan

\* These papers were unavailable at the time of publication.