

American Chemical Society
Division of Computers in Chemistry
240th ACS National Meeting, Boston, MA, August 22-26, 2010

E. X. Esposito, Program Chair; J. D. Madura, Program Chair

SUNDAY MORNING

Proteins

E. X. Esposito, Organizer; V. Somiseti, Presiding Papers 1-6

Colloids: Gels, Sols, and Emulsions. You Know... Goo

E. X. Esposito, Organizer; K. Armacost, Presiding Papers 7-12

Tautomers and Biology

T. Stouch, Organizer; Y. Martin, Organizer; T. Stouch, Presiding Papers 13-17

Methodology for Small Systems

E. X. Esposito, Organizer; V. Pakkala, Presiding Papers 18-22

Drug Discovery

S. Wildman, Organizer; Y. Tseng, Organizer; Z. Yang, Presiding Papers 23-28

Novel Is So Passé, Just Say NEW Methods

E. X. Esposito, Organizer; S. Kim, Presiding Papers 29-35

Frontiers of Condensed Phase Theory and Simulation: A Tribute to Bruce J. Berne

G. Voth, Organizer; J. Straub, Organizer; M. Tuckerman, Organizer; M. Tuckerman, Presiding Papers 36-41

SUNDAY AFTERNOON

Frontiers of Condensed Phase Theory and Simulation: A Tribute to Bruce J. Berne

G. Voth, Organizer; J. Straub, Organizer; M. Tuckerman, Organizer; P. Rossky, Presiding Papers 42-47

Proteins

E. X. Esposito, Organizer; H. Liu, Presiding Papers 48-54

Scripting & Programming

R. Guha, Organizer; R. Guha, Presiding Papers 55-61

The PDB and Chemistry

T. Stouch, Organizer; T. Stouch, Presiding Papers 62-68

Drug Discovery

S. Wildman, Organizer; Y. Tseng, Organizer; P. Mukherjee, Presiding Papers 69-75

Using Waters Explicitly in Drug Discovery

V. Shanmugasundaram, Organizer; W. Sherman, Organizer; W. Sherman, Presiding Papers 76-81

We Were Promised Jet Packs. They Found Out About These on the Way

E. X. Esposito, Organizer; Z. Cournia, Presiding Papers 82-88

MONDAY MORNING

Frontiers of Condensed Phase Theory and Simulation: A Tribute to Bruce J. Berne

G. Voth, Organizer; J. Straub, Organizer; M. Tuckerman, Organizer; J. Cao, Presiding Papers 89-94

An Emerging Challenge in Multiscale Modeling and Simulation: Mechanistic Understandings

H. Guo, Organizer; J. Chu, Organizer; J. Chu, Presiding Papers 95-100

Tautomers and Biology

T. Stouch, Organizer; Y. Martin, Organizer; Y. Martin, Presiding Papers 101-106

Drug Discovery

S. Wildman, Organizer; Y. Tseng, Organizer; S. Natesan, Presiding Papers 107-111

Waters: Feisty Little Molecules

E. X. Esposito, Organizer; K. Immadisetty, Presiding Papers 112-117

Challenges in Industrial Computational Methods

A. Nicholls, Organizer; E. Sourial, Organizer; C. Lemmen, Presiding; C. Groom, Presiding Papers 118-119

The Community Structure-Activity Resource (CSAR) Scoring Challenge

H. Carlson, Organizer; H. Carlson, Presiding Papers 120-124

MONDAY AFTERNOON

Frontiers of Condensed Phase Theory and Simulation: A Tribute to Bruce J. Berne

G. Voth, Organizer; J. Straub, Organizer; M. Tuckerman, Organizer; R. Silbey, Presiding Papers 125-130

An Emerging Challenge in Multiscale Modeling and Simulation: Mechanistic Understandings

H. Guo, Organizer; J. Chu, Organizer; M. Hagan, Presiding Papers 131-136

Challenges in Industrial Computational Methods

A. Nicholls, Organizer; E. Sourial, Organizer; C. Lemmen, Presiding; C. Groom, Presiding Papers 137-138

The Journal of Chemical Information and Modeling's 50th Anniversary Symposium

W. Jorgensen, Organizer; W. Jorgensen, Presiding Papers 139-144

The Community Structure-Activity Resource (CSAR) Scoring Challenge

H. Carlson, Organizer; J. Dunbar, Presiding Papers 145-150

Using Waters Explicitly in Drug Discovery

V. Shanmugasundaram, Organizer; W. Sherman, Organizer; V. Shanmugasundaram, Presiding Papers 151-157

MONDAY EVENING

Sci-Mix

E. X. Esposito, Organizer Papers 233, 242, 237, 243, 256, 249, 266, 257, 255, 288, 268, 271, 307, 296, 302

TUESDAY MORNING

Frontiers of Condensed Phase Theory and Simulation: A Tribute to Bruce J. Berne

G. Voth, Organizer; J. Straub, Organizer; M. Tuckerman, Organizer; H. Stern, Presiding Papers 158-163

An Emerging Challenge in Multiscale Modeling and Simulation: Mechanistic Understandings

H. Guo, Organizer; J. Chu, Organizer; J. Chu, Presiding Papers 164-169

Tautomers and Biology

T. Stouch, Organizer; Y. Martin, Organizer; Y. Martin, Presiding Papers 170-173

The Community Structure-Activity Resource (CSAR) Scoring Challenge

H. Carlson, Organizer; H. Carlson, Presiding Papers 174-177

Drug Discovery

S. Wildman, Organizer; Y. Tseng, Organizer; R. Baron, Presiding Papers 178-184

Quantum Chemistry

E. X. Esposito, Organizer; J. Sanders, Presiding Papers 185-188

Challenges in Industrial Computational Methods

A. Nicholls, Organizer; E. Sourial, Organizer; C. Lemmen, Presiding; C. Groom, Presiding Papers 189-190

TUESDAY AFTERNOON

Frontiers of Condensed Phase Theory and Simulation: A Tribute to Bruce J. Berne

G. Voth, Organizer; J. Straub, Organizer; M. Tuckerman, Organizer; J. Skinner, Presiding Papers 191-196

An Emerging Challenge in Multiscale Modeling and Simulation: Mechanistic Understandings

H. Guo, Organizer; J. Chu, Organizer; W. Noid, Presiding Papers 197-202

Challenges in Industrial Computational Methods

A. Nicholls, Organizer; E. Sourial, Organizer; C. Lemmen, Presiding; C. Groom, Presiding Papers 203-204

Insane in the Membrane

E. X. Esposito, Organizer; S. Manepalli, Presiding Papers 205-211

Docking & Scoring: What Have We Learned and Where Are We Now?

N. Nevins, Organizer; G. Warren, Organizer; G. McGaughey, Organizer; G. McGaughey, Presiding Papers 212-216

Using Waters Explicitly in Drug Discovery

V. Shanmugasundaram, Organizer; W. Sherman, Organizer; W. Sherman, Presiding Papers 217-223

TUESDAY EVENING

Chemical Computing Group Excellence Award

C. Simmerling, Organizer Papers 224-228

Hewlett-Packard Outstanding Junior Faculty Award

C. Simmerling, Organizer Papers 229-232

Poster Session

E. X. Esposito, Organizer Papers 233-316

WEDNESDAY MORNING

Frontiers of Condensed Phase Theory and Simulation: A Tribute to Bruce J. Berne

G. Voth, Organizer; J. Straub, Organizer; M. Tuckerman, Organizer; J. Straub, Presiding Papers 317-322

An Emerging Challenge in Multiscale Modeling and Simulation: Mechanistic Understandings

H. Guo, Organizer; J. Chu, Organizer; P. Liu, Presiding Papers 323-328

Success Stories in Computer-Guided Chemistry

A. Parrill, Organizer; A. Parrill, Presiding Papers 329-334

Docking & Scoring: What Have We Learned and Where Are We Now?

G. McGaughey, Organizer; G. Warren, Organizer; N. Nevins, Organizer; G. McGaughey, Presiding Papers 335-340

Drug Discovery

S. Wildman, Organizer; Y. Tseng, Organizer; A. Patny, Presiding Papers 341-345

Challenges in Industrial Computational Methods

A. Nicholls, Organizer; E. Sourial, Organizer; C. Lemmen, Presiding; C. Groom, Presiding Papers 346

WEDNESDAY AFTERNOON

Frontiers of Condensed Phase Theory and Simulation: A Tribute to Bruce J. Berne

G. Voth, Organizer; J. Straub, Organizer; M. Tuckerman, Organizer; G. Voth, Presiding Papers 347-352

An Emerging Challenge in Multiscale Modeling and Simulation: Mechanistic Understandings

H. Guo, Organizer; J. Chu, Organizer; H. Guo, Presiding Papers 353-358

Scripting & Programming

E. Fluder, Organizer; Z. Yang, Organizer Papers 359-362

Docking & Scoring: What Have We Learned and Where Are We Now?

N. Nevins, Organizer; G. Warren, Organizer; G. McGaughey, Organizer Papers 363-368

Emerging Technologies in Computational Chemistry

C. Breneman, Organizer; C. Breneman, Presiding Papers 369-375

THURSDAY MORNING

Targeting Gram-Negative Pathogens

V. Shanmugasundaram, Organizer; J. Starr, Organizer; V. Shanmugasundaram, Presiding Papers 376-382

Materials, Polymers, and Nano-stuff

E. X. Esposito, Organizer; J. Kelley, Presiding Papers 383-388

An Emerging Challenge in Multiscale Modeling and Simulation: Mechanistic Understandings

H. Guo, Organizer; J. Chu, Organizer; H. Guo, Presiding Papers 389-394

Peter McWilliams said, 'Life is Not a Struggle. It's a Wiggle.'

E. X. Esposito, Organizer; D. Xu, Presiding Papers 395-401

CANCELLED Docking & Scoring: What Have We Learned and Where Are We Now?

N. Nevins, Organizer; G. McGaughey, Organizer; G. Warren, Organizer; G. Warren, Presiding Papers 402-407

Drug Discovery

S. Wildman, Organizer; Y. Tseng, Organizer; J. Jansen, Presiding Papers 408-414

THURSDAY AFTERNOON

An Emerging Challenge in Multiscale Modeling and Simulation: Mechanistic Understandings

H. Guo, Organizer; J. Chu, Organizer; X. Huang, Presiding Papers 415-418

Targeting Gram-Negative Pathogens

V. Shanmugasundaram, Organizer; J. Starr, Organizer; J. Starr, Presiding Papers 419-426

Materials, Polymers, and Nano-stuff

E. X. Esposito, Organizer; R. Paton, Presiding Papers 427-432

Data Analysis: Statistics on Chemicals

E. X. Esposito, Organizer; A. Abebe, Presiding Papers 433-438

CANCELLED Docking & Scoring: What Have We Learned and Where Are We Now?

N. Nevins, Organizer; G. McGaughey, Organizer; G. Warren, Organizer; G. Warren, Presiding Papers 439-445

Drug Discovery

S. Wildman, Organizer; Y. Tseng, Organizer; R. Napoleon, Presiding Papers 446-450