

SYMPOSIUM CM3

Computer-Based Modeling and Experiment for the Design
of Soft Materials
April 18 - April 21, 2017

Symposium Organizers

Peter Coveney, University College London
Valeriy Ginzburg, Dow Chemical Company
Olga Kuksenok, Clemson University
Veena Tikare, Sandia National Laboratories

Symposium Support

Clemson University, Department of Materials Science and
Engineering
Goodyear Tire and Rubber Company
PPG Industries, Inc.
Sandia National Laboratories
The Dow Chemical Company

Proceedings Statement

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* Invited Paper

SESSION CM3.1: Gels, Biopolymers and Active Matter
Session Chairs: Peter Coveney and Russell Thompson
Tuesday Morning, April 18, 2017
PCC North, 100 Level, Room 127 A

10:30 AM *CM3.1.01

Surface-Bound Enzymatic Reactions Organize Microcapsules and Protocells in Solution [Anna C. Balazs](#); University of Pittsburgh, United States.

11:00 AM CM3.1.02

Magnonics in Hydrogels—Modeling Magnetomechanical Effects in GHz Frequency Range [Olga Kuksenok](#); Clemson University, United States.

11:15 AM *CM3.1.03

Mesoscale Modelling of Active Matter [Julia M. Yeomans](#); University of Oxford, United Kingdom.

11:45 AM CM3.1.04

Understanding Micromechanics of Stimuli-Sensitive Microgels Using Dissipative Particle Dynamics [Alexander Alexeev](#); Georgia Institute of Technology, United States.

SESSION CM3.2: Polymers for Water, Energy and Separations—Membranes, Porous Materials and Foams

Session Chairs: Alexander Alexeev and Olga Kuksenok
Tuesday Afternoon, April 18, 2017
PCC North, 100 Level, Room 127 A

1:30 PM *CM3.2.01

From Toy Models to Materials Models—Integrating Experiment-Specific Morphologies in Mesoscale Simulations of Porous Media [Ulf D. Schiller](#); Clemson University, United States.

2:00 PM CM3.2.02

Development of Laminar Graphene Oxide Water Separation Membrane Using Computer Simulation and Experiment [Ram Devanathan](#); Pacific Northwest National Laboratory, United States.

2:15 PM *CM3.2.03

Developing New Nanoporous Materials for Practical Applications Using Computational Modeling—How Close is the Dream to Reality? [David Sholl](#); Georgia Institute of Technology, United States.

2:45 PM BREAK

3:15 PM *CM3.2.04

Self-Assembly and Transport in Polyelectrolyte Membranes [Alexander V. Neimark](#); Rutgers University, United States.

3:45 PM CM3.2.05

A Predictive Equation of State for Solubilities—Nanocellular Polymeric Foams and Hydrogen Storage Applications [Russell B. Thompson](#); University of Waterloo, Canada.

4:00 PM CM3.2.06

Simple Coarse-Grained Modeling of Regioregularity Controlled P3HT Molecules [YongJoo Kim](#); KAIST, Korea (the Republic of).

4:15 PM CM3.2.07

Coarse-Grained Forcefield for Mesoscale Interface Morphology Design in Polymer Solar Cells [Meilin Li](#)^{1,2}; ¹National University of Singapore, Singapore; ²Solar Energy Research Institute of Singapore, Singapore.

4:30 PM CM3.2.08

Multiscale Modeling of Carbon Nanotube Bundle Agglomeration inside a Gas Phase Pyrolysis Reactor [Guangfeng Hou](#); University of Cincinnati, United States.

4:45 PM CM3.2.09

Effect of pH on the Interfacial Properties of Silicate Glasses [Ross J. Stewart](#); Corning Inc., United States.

SESSION CM3.3/CM7.2: Joint Session: Accelerating Materials Discovery and Design with Computing

Session Chairs: Alexander Alexeev and Veena Tikare
Wednesday Morning, April 19, 2017
PCC North, 100 Level, Room 124 B

8:00 AM *CM3.3.01/CM7.2.01

NIST—The Materials Genome Initiative and Computation [James A. Warren](#); National Institute of Standards and Technology, United States.

8:30 AM CM3.3.02/CM7.2.02

Intelligently Navigating Parameter Space with Machine Learning [Matthew Spellings](#); University of Michigan, United States.

8:45 AM CM3.3.03/CM7.2.03

Materials Data Management with Signac [Carl Simon Adorf](#); University of Michigan, United States.

9:00 AM CM3.3.04/CM7.2.04

Digital Alchemy—An Inverse Approach to Mesoscale Soft Materials Design [Greg van Anders](#); University of Michigan, United States.

9:15 AM CM3.3.05/CM7.2.05

Pressure-Induced Phase Transitions in Shape Space [Rose Cersonsky](#); University of Michigan, United States.

9:30 AM CM3.3.06/CM7.2.06

Determining Molecular Orientation via Physics Based Polymer Models with Polarized X-Ray Scattering [Adam F. Hannon](#)^{1,2}; ¹NIST, United States; ²Georgetown University, United States.

9:45 AM BREAK

10:15 AM *CM3.3.07/CM7.2.07

Evolutionary Structure Prediction from Complex Crystals to Defects [Qiang Zhu](#); University of Nevada, Las Vegas, United States.

10:45 AM CM3.3.08/CM7.2.08

Large-Scale Molecular Dynamics Simulation on Fracture Properties of Ni Anode for Highly Durable Solid Oxide Fuel Cell [Jingxiang Xu](#); Institute for Materials Research, Tohoku University, Japan.

11:00 AM CM3.3.09/CM7.2.09

Integrated Imaging and Simulation to Investigate Lattice Deformations in Externally Stimulated Nanocrystals Kiran Sasikumar; Argonne National Laboratory, United States.

11:15 AM CM3.3.10/CM7.2.10

DFT Applied to Transition Metals and Binaries—Developing the V/DM-17 Test Set Elizabeth Decolvenaere; University of California, Santa Barbara, United States.

11:30 AM CM3.3.11/CM7.2.11

Development of Crystal Structure Prediction Method for Magnet Materials Tomoki Yamashita^{1,2}; ¹National Institute for Materials Science (NIMS), Japan; ²Osaka University, Japan.

SESSION CM3.4: Industrial Applications of Polymer Modeling I

Session Chairs: Valeriy Ginzburg and Russell Thompson

Wednesday Afternoon, April 19, 2017

PCC North, 100 Level, Room 127 A

1:30 PM *CM3.4.01

Towards Accelerated Materials Discovery and Design Turab Lookman; Los Alamos National Laboratory, United States.

2:00 PM *CM3.4.02

Modelling at the Appropriate Lengthscale for Industrial Applications Massimo Noro; Unilever, United Kingdom.

2:30 PM BREAK

3:30 PM *CM3.4.03

Stimuli Interactive Materials: Making Materials Locomote Richard A. Vaia; Air Force Research Laboratory, United States.

4:00 PM CM3.4.04

Characterizing the Fundamental Adhesion of Polyimide on Crystalline and Glassy Silica Surfaces—A Molecular Dynamics Study Sushmit Goyal; Corning Inc, United States.

4:15 PM CM3.4.05

Computational Screening and Design of Complex Structures Julia Dshemuchadse; University of Michigan, United States.

4:30 PM CM3.4.06

Calculation of Solvation Free Energies for the Predictive Design of Functional Molecular Systems Wenkun Wu; University of Michigan, United States.

4:45 PM CM3.4.07

Microstructural Quantification and Property Prediction Using Limited X-Ray Tomography Data Yang Jiao; Arizona State University, United States.

SESSION CM3.5: Poster Session: Computer-Based Modelling and Experiment for the Design of Soft Materials

Session Chairs: Peter Coveney, Valeriy Ginzburg, Olga Kuksenok and Veena Tikare

Wednesday Afternoon, April 19, 2017

8:00 PM - 10:00 PM

Sheraton, Third Level, Phoenix Ballroom

CM3.5.01

Morphological Control—A Correlation between Theoretical and Experimental Findings on Ag₂CrO₄ Microcrystals Gabriela S. Silva; Federal University of São Carlos, Brazil.

CM3.5.02

The Theoretical Engineering and Experimental Synthesis of Molecularly Imprinted Polymers as More Specific Potential Platforms for Chemical Sensing Ghada A. Selim; American University in Cairo, Egypt.

CM3.5.03

Modelling the Effect of Copolymer Concentration on Thermal Stability of Lysozyme-Copolymer Conjugates Chandan K. Choudhury; Clemson University, United States.

CM3.5.04

Simulative Study on Vaporization Condition of OMCTS by COMSOL for SiO₂ Clean Production Jun Ho Lee; Kumoh National Institute of Technology, Korea (the Republic of).

CM3.5.05

Coupling Experimental Results and Computational Models to Evaluate Peptide-Surface Interactions Kristi Singh; Air Force Research Laboratory, United States.

SESSION CM3.6: Industrial Applications of Polymer Modeling II

Session Chairs: Veena Tikare and Qiang Wang

Thursday Morning, April 20, 2017

PCC North, 100 Level, Room 127 A

8:00 AM *CM3.6.01

Atomistic and Coarse-Grained Simulations of Ion-Conducting Polymers Amalie L. Frischknecht; Sandia National Labs, United States.

8:30 AM CM3.6.02

Prediction of Phase Diagram in Thermoset/Thermoplastic Mixtures Chunyu Li; Purdue University, United States.

8:45 AM CM3.6.03

Advanced Understanding of Paper Coating Structure and Its Relationship to Coating Performance Jian Yang; The Dow Chemical Company, United States.

9:00 AM CM3.6.04

Inelastic Neutron Scattering Analysis of Polymorphic Crystals Bruce S. Hudson; Syracuse University, United States.

9:15 AM CM3.6.05

Modeling Thermal Conductivity of Polymer-Ceramic Composites by Using Scanning Electron Microscopy Images as Input to Finite Element Analysis Ellen Keene; The Dow Chemical Company, United States.

9:30 AM CM3.6.06

Modeling the Dynamical Mechanical Behavior of Polyurethane Elastomers by Combining Self-Consistent Field Theory (SCFT) and Finite Element Analysis (FEA) Valeriy V. Ginzburg; Dow Chemical Co, United States.

9:45 AM BREAK

10:15 AM *CM3.6.07

Computational Fluid Dynamics Modeling of Viscoelastic Droplet Breakup Laura J. Dietsche; The Dow Chemical Company, United States.

10:45 AM CM3.6.08

Computing Memory Effects in Coarse-Grained Modeling Derived from the Mori-Zwanzig Formalism—Application to Polymer Melts Zhen Li; Brown University, United States.

11:00 AM CM3.6.09

Systematic and Simulation-Free Coarse Graining of Polymer Melts Qiang Wang; Colorado State University, United States.

11:15 AM CM3.6.10

Modeling the Interaction of Magnetically Capped Colloidal Particles Gemming Sibylle^{1,2}; ¹Helmholtz-Zentrum Dresden-Rossendorf, Germany; ²Technische Universität Chemnitz, Germany.

11:30 AM CM3.6.11

Using Molecular Dynamics in Modeling Fluorescent Rosette Nanotubes Arthur A. Gonzales III; Northeastern University, United States.

11:45 AM CM3.6.12

Parametric Study for Dimeric Anthracene-Based Mechanophore-Embedded Thermoset Polymer Matrix Using Molecular Dynamics Bonsung Koo; Arizona State University, United States.

SESSION CM3.7: Polymer-Based Composites and Nanocomposites

Session Chairs: Peter Coveney and Reid Van Lehn

Thursday Afternoon, April 20, 2017

PCC North, 100 Level, Room 127 A

1:30 PM *CM3.7.01

Understanding Nanoconfinement and Nanoscale Interfaces in Structural Materials [Sinan Keten](#); Northwestern University, United States.

2:00 PM CM3.7.02

Detailed Investigation of Interfacial Molecular Interactions for Graphene-Based Rubber Nanocomposites [Jeeno Jose](#); Indian Institute of Technology Madras, India.

2:15 PM CM3.7.03

Modeling Isolated Polymer-Grafted Nanoparticles on Surfaces—Effect of Adsorption Strength on Morphology and Dynamics [Jeffrey Ethier](#); Ohio State University, United States.

2:30 PM *CM3.7.04

Utilizing Multiscale Modeling in Elastomer Composite Research for Tire Applications [George Papakonstantopoulos](#); Goodyear Tire and Rubber, United States.

3:00 PM BREAK

3:30 PM CM3.7.05

An Adaptive Design Approach for Exploring the Interphase Properties in Polymer Nanocomposites [Yixing Wang](#); Northwestern University, United States.

3:45 PM CM3.7.06

Properties and Processing of Clay-Polymer Nanocomposites Modelled Using a Multiscale Approach [James Suter](#); University College London, United Kingdom.

4:00 PM CM3.7.07

New Insights into Graphene Exfoliation with Molecular Dynamics [Robert Sinclair](#); University College London, United Kingdom.

4:15 PM CM3.7.08

Modelling the Viscoelastic Properties of Polymer Nanocomposites [Merabia Samy](#); Universite de Lyon, CNRS, UCBL, ILM, UMR5306, France.

SESSION CM3.8: Liquid Crystals, Colloids and Granular Materials

Session Chairs: Valeriy Ginzburg and Qiang Wang

Friday Morning, April 21, 2017

PCC North, 100 Level, Room 127 A

8:00 AM *CM3.8.01

Object Oriented Programming with Liquid Crystals [Randall D. Kamien](#); University of Pennsylvania, United States.

8:30 AM CM3.8.02

Geometry of Tubular Crystals Containing Topological Defects [Daniel Beller](#); Harvard University, United States.

8:45 AM CM3.8.03

Phase Transition in Plastic Crystalline Assemblies of Janus Colloids—Similarities with Isotropic-Nematic Liquid Crystals [Hossein Rezvantalab](#); University of Michigan, United States.

9:00 AM CM3.8.04

Design of Membrane-Embedded Amphiphilic Nanoparticles from Multiscale Simulations [Reid Van Lehn](#); University of Wisconsin-Madison, United States.

9:15 AM CM3.8.05

Experimental and Computational Characterization of Wet Granular Media [Hosain Bagheri](#); Arizona State University, United States.

9:30 AM CM3.8.06

Heterogeneous Nanomechanical Properties of Type I Collagen in the Longitudinal Direction [Ming Tang](#); Queensland University of Technology, Australia.

9:45 AM BREAK

10:15 AM *CM3.8.07

Constructing Novel Polymorphs from Predicted Nanoclusters Taken from the Hive [Scott M. Woodley](#); University College London, United Kingdom.

10:45 AM CM3.8.08

Experimental and Computational Characterization of Granular Media at Microgravity with Electrostatic Forces [Andrew L. Thoesen](#); Arizona State University, United States.

11:00 AM CM3.8.09

Design of Origami-Based Mechanical Instabilities to Amplify Active Material Responses [Phil Buskohl](#); Air Force Research Laboratory, United States.

11:15 AM CM3.8.10

Diffusion of Water into Biopolymer Matrix under Different Mechanical Strain [Santhosh Mathesan](#); Indian Institute of Technology Madras, India.

11:30 AM CM3.8.11

Computational Design of Biomimetic Nanoparticles for Nucleic Acid Packaging [Jessica Nash](#); North Carolina State University, United States.

11:45 AM CM3.8.12

Improving Thermal Stability of Hen Egg White Lysozyme via Conjugation with Copolymer [Chandan K. Choudhury](#); Clemson University, United States.

SESSION CM3.9: New Modeling Approaches on Multiple Length Scales

Session Chairs: Olga Kuksenok and Reid Van Lehn

Friday Afternoon, April 21, 2017

PCC North, 100 Level, Room 127 A

1:30 PM *CM3.9.01

Multiscale by Focusing on Bridging between Established Fields and Codes [Ann E. Mattsson](#); Sandia National Laboratories, United States.

2:00 PM CM3.9.02

Effect of Graphene Oxidation on Structure and Dynamics of Biomolecules Using Computational Modeling [Hoshin Kim](#); North Carolina State University, United States.

2:15 PM CM3.9.03

Incorporating Complex Reaction Mechanisms into Classical Molecular Dynamics [Jacob Gissinger](#); University of Colorado-Boulder, United States.

2:30 PM *CM3.9.04

Multiscale Modelling of Nanoscale Materials and Electronic Transport [Wolfgang Wenzel](#)^{1,2}; ¹Karlsruhe Institute of Technology, Germany; ²Nanomatch GmbH, Germany.

3:00 PM BREAK

3:30 PM CM3.9.05

DFT and Force Field Study on the Effect of Ions on Structure and Side-Chain Interactions in Peptoids [Marcel D. Baer](#); PNNL, United States.

3:45 PM CM3.9.06

Phosphorescence from Pure Organic Bromofluorene Derivatives—Simulation and Experimental Studies [Hossein Hashemi](#); University of Michigan, United States.

4:00 PM CM3.9.07

Peptide Coated Gold Cluster Designed as Target Probe by Computational and Experimental Methods [Lina Zhao](#); Institute of High Energy Physics, Chinese Academic Sciences, China.

4:15 PM CM3.9.08

Mesoscale Modeling of Peptide Nanotube [Leela Rakesh](#); Central Michigan University, United States.

4:30 PM CM3.9.09

Magneto-Elastic Colloidal Membranes [Mykola Tasinkevych](#); Northwestern University, United States.