## PRESENTATIONS

Invited Talks in Scientific Meetings

"Atomistic Simulations of Structure and Mechanical Properties of Polymeric Glasses", Polymer Design and Simulation Consortium-Winter 1988, Pasadena, California, February 1988.

"Data and Knowledge for Materials Design", talk and panel discussion, Alcoa Laboratories Technical Symposium on Opportunities for Computer Science to Advance Material Science, Nemacolin, Pennsylvania, October 1989.

"Molecular Modeling of Polymers at Interfaces", BIOSYM Seminar on Computer Simulation of Polymers and Polymeric Systems, Irvine, Texas, April 1990.

"Molecular Modeling of Polymers at Interfaces", BIOSYM Polymer Project Consortium Meeting, Paris, France, June 1990.

"Molecular Modeling of Interfacial Structure and Thermodynamics of Polymers", Third Workshop of the American Chemical Society on Polymer Surfaces and Interfaces, Asilomar Conference Center, Pacific Grove, California, October 1990.

"Molecular Modeling of Polymers at Interfaces", Symposium on Models for Polymer Thermodynamics, 1990 Annual Meeting of the American Institute of Chemical Engineers, Chicago, Illinois, November 1990.

"Determination of Gas Separation Properties of Zeolites from Molecular-level Information by Supercomputation", Engineering Foundation Fourth International Conference on Separation Technology, Kona, Hawaii, October 1991.

"Molecular Modeling of Amorphous Polymers in the Bulk and at Interfaces", Shell Conference on the Prediction of Polymer Physical Properties: Status and Perspectives, Château Marquette, Heemskerk, The Netherlands, November 1991.

"Structure and Dynamics of Polymers at Interfaces", 1992 Moretonhampstead Polymer Science Meeting on Polymer Science and Technology Signposts for the Future, Moretonhampstead, England, April 1992.

"Molecular Modeling of Adsorption and Transport in Zeolite Molecular Sieves", The 39th Gordon Research Conference on Separation and Purification, New London, New Hampshire, August 1992.

"Molecular Modeling of Polymers at Interfaces", International Polymer Simulation Conference sponsored by Molecular Simulations Inc., Reading, England, September 1992.

"Atomistic Simulations of Structure and Molecular Motion in a Glassy Polymer", 2nd International Discussion Meeting on Relaxations in Complex Systems, Alicante, Spain, July 1993.

"A Strategy for Atomistic Monte Carlo Simulations of Polydisperse Polymer Systems", ACS Division of Polymer Chemistry Symposium on Polymer Dynamics and Thermodynamics in Solutions in honor of Professor Walter H. Stockmayer, San Diego, California, March 1994.

"Molecular Modeling of Amorphous Polymer Properties", Gordon Research Conference on Polymers, Brewster Academy, Wolfeboro, New Hampshire, July 1994.

"Atomistic Modeling of Amorphous Polymers: Promises and Challenges", First Australian Workshop on Molecular Simulation of Polymers, Austalian National University, Canberra, ACT, Australia, September 1994.

"Modeling Structure and Adhesion at Polymer/Copolymer/Polymer Interfaces", ACS Interdisciplinary Workshop on Polymer Surfaces and Interfaces, Brewster, Massachusetts, October 1994.

"Monte Carlo Strategies for the Prediction of Properties of Polymer Glasses and Melts", 5th European Polymer Federation Symposium on Polymeric Materials, Basel, Switzerland, October 1994.

"Molecular Modeling of Polymer/Solid and Polymer/Polymer Interfaces, keynote lecture, International Conference on Interfacial Phenomena in Composite Materials, Eindhoven, The Netherlands, September 1995.

"Molecular Simulations of Long-Chain Alkanes in Zeolite Pores", Symposium: Moleküle in Wechselwirkung mit Grenzflächen, Universität Leipzig, September 1995.

"Atomistic Simulations of Amorphous Polymers", Greek-French Polymer Workshop, FORTH, Heraklion, Crete, Greece, May 1996.

"Monte Carlo Approaches for Equilibrating Amorphous Polymer Systems", Monte Verità Conference on Structural and Dynamic Modeling of Mechanical Behaviour of Solids, Ascona, Switzerland, September 1996.

"From Chemical Structure to the Physical Properties of Polymer Systems: What Do Theory and Molecular Simulations Have to Offer?" 12th Panhellenic Conference on Solid State Physics, Heraklion, Crete, Greece, September 1996.

‘‘Prediction of Sorption and Diffusion of Hydrocarbons in Zeolites through New, Hierarchical Molecular Simulation Techniques’’, Symposium on Advances and Applications of Computational Chemical Modeling to Heterogeneous Catalysis, 213$^{th}$ ACS National Meeting, San Francisco, California, April 1997.

‘‘New Atomistic Simulation Approaches for the Prediction of Relaxation Phenomena in Polymer Melts’’, 3$^{rd}$ International Discussion Meeting on Relaxations in Complex Systems, Vigo, Spain, June 1997.

‘‘Small Molecule Diffusion in Amorphous Polymers’’, Enrico Fermi Summer School on the Computer Simulation of Rare Events and the Dynamics of Classical and Quantum Condensed Systems, Lerici, Italy, July 1997.

‘‘Hierarchical Modeling Strategies for Polymer Melts and Glasses: Elasticity, Viscosity, and Interfacial Fracture’’, CECAM discussion meeting on Multiscale Modeling and Grand Challenge Problems in Materials Research, Lyon, France, October 1997.

‘‘Efficient Monte Carlo Strategies for the Equilibration of Atomistic Models of Chain Fluids’’, CECAM Workshop on Algorithms for Simulating Complex Molecular Systems, Lyon, France, April 1998.

‘‘Prediction of Elasticity and Viscosity of Long-chain Polymer Melts through New, Efficient Atomistic Simulation Strategies’’, keynote lecture, Symposium on Molecular Simulation of Polymer Systems, World Polymer Congress Macro 98, Gold Coast, Australia, July 1998.

‘‘Molecular Modeling of Materials’’, invited presentation and participation in the annual conference *Scientia Europaea*, organised by the Institut de France and the Fondation Rhône-Poulenc, Pornichet, France, September 1998.

‘‘Simulation of Diffusion in Zeolites’’, international workshop ‘Integrating Zeolite Science and Technology’, Royal Netherlands Academy of Arts and Sciences, Amsterdam, October 1998.

‘‘Mechanism and Rates of Small-Molecule Diffusion in Amorphous Polymers as Revealed by Molecular Dynamics and Transition-State Theory Calculations’’, 2nd International Workshop on Molecular Modeling in Membrane Research, Teltow, Germany, March 1999.

‘‘Molecular Simulations of Diffusion in Polymers’’, European Research Conference on Catalysis in Membrane Reactors, Ravello, Italy, May 1999.

‘‘Coarse-Grained Modeling of Adhesion at Polymer-Polymer Interfaces Strengthened With Graft Copolymers’’, CECAM-ESF Workshop on Computer Simulations of Polymer Blends and Copolymer Systems, Lyon, France, September 1999.

‘‘Connectivity-altering Algorithm for the Fast Equilibration of Dense Polymer Systems’’, CECAM Workshop on Overcoming Broken Ergodicity in Simulations of Condensed Matter Systems, Lyon, France, September 1999.

‘‘Hierarchical Modeling of Structure and Adhesion at Polymer/Polymer Interfaces’’, European Research Conference on Interfaces and Colloidal Systems, Aghia Pelaghia, Crete, Greece, Sept. 1999.

‘‘Simulations of Alkanes and Their Mixtures in Silicalite Pores’’, CECAM Workshop on Transport Behavior of Guest Molecules in Zeolites, Lyon, France, October 1999.

‘‘Hierarchical Simulation Schemes for the Prediction of Polymer Material Properties’’, 11th Royal Australian Chemical Institution Convention – Chemistry into the New Millennium, Canberra, Australia, February 2000.

‘‘Infrequent-event analysis of structural relaxation in a Lennard-Jones glass’’, CECAM Workshop on Characterizing and Studying Transition Mechanisms and States in High-Dimensional Systems, Lyon, France, May 2000.

‘‘Calculation of gas diffusivity in a glassy polymer based on multidimensional transition-state theory’’, CECAM-SIMU Workshop on Characterizing and Studying Transition Mechanisms and States in High-Dimensional Systems, Lyon, France, May 2000.

‘‘Property Prediction Through Molecular Simulation: Status and Perspectives’’, 18th European Seminar on Applied Thermodynamics, Kutná Hora, Czech Republic, June 2000.

‘‘Segmental Dynamics in Polymer Melts and Blends: Computer Simulations Confronted With Experimental Measurements’’ Workshop on Future Perspectives for Understanding the Unsolved Problem of the Glass Transition by Neutron Scattering and Computer Simulation, Donostia Physics Center, San Sebastián, Spain, June 2000.

‘‘Structural Relaxation in Amorphous Solids as a Sequence of Jumps in Configuration Space’’, CECAM-SIMU Workshop on Simulations of Long Time Scale Dynamics, Molecular and Continuum Descriptions, Reykjavík, Iceland, June 2000.

‘‘Hierarchical Schemes for Calculating Polymer Physical Properties’’, SIMU Workshop on Multiscale Modeling of Macromolecular Systems, MPI für Polymerforschung, Mainz, Germany, September 2000.

‘‘Hierarchical Modeling of Rheological, Permeability, and Adhesion Properties of Polymers’’, MML2000 International Workshop on Materials Modeling: Across the Length Scales II. Applications in Materials Processing. Department of Materials, University of Oxford, Sept. 2000.

‘‘Mobility of young researchers across Europe: Experiences from Participation in the TMR programme’’, Keynote lecture, European Commission conference ‘Investing in Europe’s Human Research Potential’, Hersonnisos, Crete, Greece, October 2000.

‘‘Hierarchical Strategies and New Algorithms for Modeling Polymer Structure and Properties’’, keynote lecture, MSI European Polymer Users’ Group Meeting, Leeds, UK, November 2000.

‘‘Hierarchical modeling of rheological and adhesion properties of polymers’’, Annual March Meeting of the American Physical Society, Seattle, USA, March 2001.

‘‘Prediction of Phase Equilibria in Macromolecular Systems from Atomistic Simulations’’, MSI Polymer Consortium International Meeting, Cambridge, UK, April 2001.

‘‘Hierarchical Modeling for Polymer Product Design: Prediction of Rheological, Permeability, and Adhesion Properties’’, 9$^{th}$ International Conference on Phase Equilibria for Product and Process Design, Kurashiki, Japan, May 2001.

‘‘Segmental Dynamics in Polymer Melts and Blends: Molecular Dynamics Simulations Compared to NMR and QENS Measurements’’, International Discussion Meeting on Relaxations in Complex Systems, Crete, Greece, June 2001.

‘‘Hierarchical Modeling of Rheological and Adhesion Properties of Polymers’’, European Polymer Federation Congress, Eindhoven, The Netherlands, July 2001.

‘‘Prediction of Polymer Physical Properties Through New, Connectivity Altering Monte Carlo Algorithms’’, CECAM-ESF Conference on Bridging the Time Scale Gap, Konstanz, Germany, September 2001.

‘‘Reflections on Graduate Polymer Education’’, Annual Spring Meeting of the American Chemical Society, Symposium honoring Ulrich W. Suter, April 2002.

‘‘From detailed atomistic to coarse-grained representations of polymer melts through molecular simulations’’, CECAM-SIMU Workshop on Coarse-graining in Complex Fluids, Lyon, France, May 2002.

‘‘Sorption and diffusion of alkanes in polyethylene: Molecular simulations compared to free volume and Rouse theory predictions’’, 3rd International Workshop on “Molecular Modeling in Membrane Research”, GKSS, Teltow, Germany, May 2002.

‘‘Hierarchical Modeling of Polymers’’, Liblice Conference on the Statistical Mechanics of Liquids, Špindlerův Mlýn, Czech Republic, June 2002.

“Modeling Structure and Adhesion at Polymer/Polymer Interfaces”, International Symposium on Chain Molecules at Interfaces: Self-Consistent Field Theory and Experiment, Wageningen, The Netherlands, August 2002.

“Polymers at Surfaces and Interfaces”, two 2-hour lectures given at the NATO Advanced Study Institute and Euroconference on Computer Simulations of Surfaces and Interfaces, Varna, Bulgaria, September 2002.

“From Molecular Structure to the Physical Properties of Polymers Through New Computational Methods”, 19th Panhellenic Chemistry Conference, University of Crete, Heraklion, Greece, November 2002.

“Hierarchical Modeling of Polymer Properties: Meeting the Challenge of Long Time Scales”, Gordon Conference “CAE in Polymer Processing”, Ventura, California, USA, March 2003.

“Computational Materials Science and Engineering: The Challenge of Bridging Length and Time Scales”, Interdisciplinary Symposium: Mathematical Modeling in Modern Technologies and Economics, NTU Athens, May 2003.

“Understanding and Predicting Structure-Property Relations in Polymeric Materials Through Molecular Simulations”, Foundations of Molecular Modeling and Simulation (FOMMS) conference, Keystone, Colorado, July 2003.

“Hierarchical Modeling of Polymers: From Atomistic Simulations to Rheological and Mechanical Properties via Entanglement Network Models”, ACS Symposium on Molecular Modeling of Macromolecules, Hilton Head Island, South Carolina, USA, March 2004.

“Connectivity-Altering Monte Carlo Algorithms for Sampling the Configuration Space of Long-Chain Polymers”, CECAM-SIMU Workshop “Accelerating Dynamical Simulations”, Lyon, France, March 2004.

“Hierarchical Modeling of Amorphous Polymers”, Conference on Computational Physics 2004 (CCP 2004), Genova, Italy, September 2004.

“Hierarchical Modeling of Polymer Physical Properties: From the Atomistic to the Macroscopic”, One-day symposium “At the Cutting-Edge of Computer Simulation – from Glasses to Cell Membranes”, organized to mark the retirement of Professor Julian H.R. Clarke, Department of Chemistry, UMIST, Manchester, UK, October 2004.

“Hierarchical Modeling of Structure-Property Relations in Polymers”, Dutch Polymer Institute (DPI) Conference “Enabling Science: Structure-Performance”, Eindhoven, The Netherlands, October 2004.

“Hierarchical Simulations of Polymeric Materials”, invited plenary lecture, Dutch Polymer Days -5 meeting, Lunteren, The Netherlands, February 2005.

"Hierarchical Modeling of Polymer Properties", International Meeting on Polymer Modeling and Its Industrial Applications", University College of Borås, Sweden, June 2005.

"Two Decades of Research in Computational Polymer Science: A Personal Perspective", invited lecture, "Day or Research" organized on the occasion of the 150th anniversary of the ETH Zürich, Zürich, Switzerland, November 2005.

"Hierarchical Modeling of Polymer Physical Properties", invited talk, "Multi-scale Modeling: Electrons, Molecules and (Bio)Materials" organized by the Dutch Academy of Sciences (KNAW), Amsterdam, April 2006.

"Atomistic and Mesoscopic Simulations of Relaxation and Plastic Deformation in Amorphous Polymers" (plenary talk), 13th International Conference on Deformation, Yield, and Fracture of Polymers, Rolduc Abbey, Kerkrade, The Netherlands, April 2006.

"Multiscale Modeling Methodologies", 4 hours of lecture in short course given after invitation by the organizers of the 3rd Annual European Rheology Conference, Crete, Greece, April 2006. Co-instructors: Kurt Kremer (MPI-P Mainz), H.C. Öttinger (ETH Zürich), M. Laso (U.P. Madrid)

"Entanglement Networks and Energy Landscapes of Amorphous Polymers" (Molecular Physics lecture), 7th Liblice Conference on the Statistical Mechanics of Liquids, Lednice, Czech Republic, June 2006.

"Hierarchical Modeling of Polymers", invited talk, 19th Panhellenic Conference and Summer School on Nonlinear Science and Complexity, Thessaloniki, July 2006.

"Hierarchical Simulations of Amorphous Polymer Properties", invited lecture, Gordon Research Conference on Polymer Physics, New London, Connecticut, July 2006.

"Hierarchical Modeling of Polymer Physical Properties", invited lecture, Multiscale Materials Modeling Conference 2006 (MMM2006), Freiburg, Germany, September 2006.

" Self-consistent Field Modeling Investigations of Polymers at Interfaces ", invited lecture, CECAM Workshop on Polymer Surfaces and Interfaces, Lyon, France, October 2006.

"Correlating Molecular Modeling and Experimental Diffusivities", invited lecture, DECHEMA-Kolloquium "New horizons for diffusion research in nanoporous materials: Experiments, Theory and Application", Frankfurt, Germany, October 2006.

"Hierarchical Modeling of Polymeric Materials", Danckwerts Lecture, Annual AIChE Meeting, San Francisco, CA, USA, November 2006.

"From Molecular Structure to Macroscopic Properties: Designing Materials to Meet the Needs of Contemporary Living", invited lecture presented at a meeting and panel discussion organized by the Bodossaki Foundation, Megaron Plus, Athens, Greece, March 2007.

"Hierarchical Modeling of Polymeric Materials", invited lecture, Scienomics Users' Meeting, NTU Athens, Greece, June 2007.

"Hierarchical Simulations of Polymers", invited lecture in the CCP5/Marie Curie Summer School "Methods in Molecular Simulation", Sheffield University, July 2007.

"Accelerating Molecular Simulations by Mapping Onto Local Energy Minima", invited lecture, Conference on Computational Physics 2007 (CCP2007), Brussels, Belgium, September 2007.

"Prediction of Physical Properties of Polymers Through Hierarchical Simulations", keynote lecture, 6th European Congress on Chemical Engineering (ECCE-6), Copenhagen, Denmark, September 2007.

"Molecular Simulations of Amorphous Polymers: Meeting the Challenge of Long Time Scales", plenary lecture, International Workshop on Molecular Modeling and Simulation in Applied Material Science, DECHEMA, Frankfurt, Germany, March 2008.

"Multiscale Simulations of Polymers: From Atomistic Models to Entanglement Networks to Rheological Properties", 5th Chemical Engineering Conference for Collaborative Research in the Eastern Mediterranean Countries, Cetraro, Italy, May 2008.

"Hierarchical Simulations of Polymers: Meeting the Challenge of Long Time Scales", 7th Liquid Matter Conference, Lund, Sweden, June 2008.

"Introduction to Statistical Mechanics and Molecular Simulation Concepts", Marie Curie Summer School on Nanostructured Materials and Membrane Modeling and Simulation (NANOMEMPRO), Patras, Greece, June 2008.

"From Chemical Structure to Physical Properties of Polymers via Hierarchical Modeling", 7th Hellenic Polymer Conference, Ioannina, September 2008.

"Progress and Outlook in Monte Carlo Simulations", Symposium "The Evolution of Molecular Modeling into a Chemical Engineering Tool", Annual AIChE meeting, Philadelphia, PA, USA, November 2008.

"Multiscale Modeling of Synthetic Polymers", Workshop on Molecular Modeling: Approaches to Computational Biophysics, National Hellenic Research Foundation, Athens, Greece, December 2008.

"Multiscale Simulations of Amorphous Polymers: Meeting the Challenge of Long Time Scales", Dick Medema Award Lecture, Dutch Polymer Days-9 Meeting, Lunteren, The Netherlands, February 2009.

"Energy Landscapes and Entanglement Networks: Molecular Simulations of the Relaxation Properties of Amorphous Properties", 14th International Conference on Deformation, Yield, and Fracture of Polymers (DYFP2009), Rolduc Abbey, Kerkrade, The Netherlands, April 2009.

"Entanglement Networks and Energy Landscapes: Molecular Simulation Approaches to the Long-Time Properties of Polymers", European Symposium on Applied Thermodynamics (ESAT-2009), Santiago de Compostela, Spain, June 2009.

"Hierarchical Simulations of Amorphous Polymers: Meeting the Challenge of Long Time Scales", 3rd Monte Verità Conference on Multiscale Modeling of Materials: Unsolved Problems and Challenges", Ascona, Switzerland, September 2009.

"Predicting Thermodynamic Properties of Polymers Through Molecular Simulation", Thomas Young Centre Plenary Lecture, Thermodynamics 2009 conference, Imperial College London, Sept. 2009.

"Meeting the Challenge of Long Time Scales in Molecular Simulations of Polymers", Jülich Soft Matter Days 2009, Bonn, Germany, November 2009.

"Molecular Modeling of Soft Matter: Meeting the Challenge of Long Time Scales", Symposium "New Frontiers in Chemical and Biochemical Engineering" honouring Professors Anastasios Karabelas and Stavros Nychas, Thessaloniki, November 2009.

"Molecular Simulations of Amorphous Polymers: The Challenge of Long Time Scales", Physical Chemistry meeting dedicated to the memory of Michael Pagitsas, Thessaloniki, Greece, April 2010.

"Simulation Strategies for Addressing the Long-Time Properties of Polymer Melts and Glasses", International Workshop "Theory and Computer Simulation of Polymers: New Developments", Moscow State University, Moscow, Russia, May 2010.

"Predicting the Separation Properties of Membrane Materials Through Molecular Simulation", Gordon Research Conference on Membranes: Materials and Processes, New London, New Hampshire, July 2010.

"Predicting Physical Properties of Polyolefins by Molecular Simulation", 8$^{th}$ Hellenic Polymer Conference (HPOL8) organized in honour of Prof. Nikos Hadjichristidis, Hersonissos, Crete, October 2010.

"Predicting the Separation Properties of Membrane Materials by Molecular Simulation", Mini-Symposium on Diffusion and Separation, CSIRO Materials Science and Engineering, Clayton, Victoria, Australia, November 2010.

"Molecular Simulations of Transport in Microporous Materials", Symposium dedicated to the memory of Alkis Payatakes, Patras, Greece, December 2010.

"Molecules in Motion: Diffusion Phenomena in Materials", Επιστήμης Κοινωνία, 4$^{th}$ cycle of lectures: Chemistry – Our Life, our Future, dedicated to the International Year of Chemistry 2011, National Hellenic Research Foundation, February 2011.

"Molecular Dynamics Investigations of the Energy Hypersurface of Glass-Forming Materials", Annual Conference of the UK Network "Mathematical Challenges in Molecular Dynamics", Imperial College London, UK, March 2011.

"Hierarchical Molecular Modeling of the Physical Properties of Polymers", Symposium "Modeling and Simulation in Polymer Product and Process Development", BASF SE Ludwigshafen, Germany, April 2011.

"Searching for Entanglements in Atomistic Simulations of Polymer Melts", Numerical Knots: Models and Simulations Workshop "Knots and Links: From Form to Function", Centro di Ricerca Matematica Ennio De Giorgi, Scuola Normale Superiore, Pisa, Italy, June 2011.

"Predicting Sorption and Diffusion in Membrane Materials by Molecular Simulation", 7th International Conference on Diffusion in Solids and Liquids (DSL 2011), Vilamoura, Portugal, June 2011.

"Multiscale Modeling of Polymer-matrix Nanocomposites", CECAM Workshop on Coarse-graining Strategies and Methodologies for Polymeric and Biomolecular Assemblies, Centre Blaise Pascal, École Normale Supérieure de Lyon, Lyon, France, July 2011.

"Coarse-graining of Polymers and Liquid Crystals with the Iterative Boltzmann Inversion Method", CECAM Workshop "Coarse-graining Methods in Self-Assembly", Lugano, Switzerland, July 2011.

"Molecular Simulations of Polyolefins: Melts, Networks, Crystals", International Workshop for Molecular Simulations of Polymers, Institute for Chemical Research, Kyoto University Gokasho, Uji, Japan, September 2011.

"Molecular Simulations of Polymer Melts and Glasses: Strategies for Meeting the Challenge of Long Time Scales", 2nd International Symposium on Multi-Scale Simulations of Biological and Soft Materials (MSBSM2011), Kyoto University, Japan, September 2011.

"Computational Materials Science: From Molecular Structure to Macroscopic Properties", Meeting to celebrate the 50 years of NCSR "Demokritos", Athens, Greece, November 2011.

"Understanding Polymer Melts and Networks Through Molecular Simulation", Annual Meeting of the Dutch Polymer Institute (DPI), Zeist, The Netherlands, November 2011.

"Tracking the Dynamics of Systems Evolving Through Infrequent Transitions in a Network of Discrete States", IAS Winter School "Hierarchical Methods for Dynamics in Complex Molecular Systems", Research Center Jülich, Germany, March 2012.

"Molecular Modeling of Cavitation in Polymer Melts and Rubbers" (with A.K. Morozinis and C. Tzoumanekas), 15$^{th}$ International Conference on Deformation, Yield, and Fracture of Polymers (DYFP2012), Rolduc Abbey, Kerkrade, The Netherlands, April 2012.

"Atomistic, Coarse-Grained, and Field Theory-Inspired Simulations of Polymer-Matrix Nanocomposites" (with Georgios G. Vogiatzis), workshop on "Computer Modeling of Polymer Nanocomposites", Lomonosov Moscow State University, June 2012.

"Multiscale Modeling of Polymer-Matrix Nanocomposites" (with Georgios G. Vogiatzis and Evangelos Voyiatzis), ACS Symposium on Computational Modeling of Polymers, ACS National Meeting, Philadelphia, PA, August 2012.

"Energy Landscape Analysis of Atomic and Polymer Glasses" (with Nikolaos Lempesis and George C. Boulougouris), Conference on Statistical Mechanics: Interplay of Theory and Computer Simulations, honouring Professor Kurt Binder, Mainz, September 2012.

"Multiscale Simulations of Polymer-Matrix Nanocomposites" (with Georgios Vogiatzis), Symposium F: Challenges in Multiscale Modeling of Biological and Soft Materials, 6th International Conference on Multiscale Materials Modeling (MMM2012), Biopolis, Singapore, October 2012.

"Computing Diffusivities in Spatially Periodic Media from the Rate Constants of Elementary Jumps Between Sorption Sites: Master Equation Solution by Recursive Reduction of Dimensionality" (with Panagiotis D. Kolokathis), Session in Honor of Alexis Bell's 70th Birthday, Annual Meeting of the AIChE, Pittsburgh, PA, October 2012.

"Chain Conformations in Polymer Nanocomposites: A Field Theory-Inspired Monte Carlo Simulation Approach" (with Georgios G. Vogiatzis), Session on Modeling and Simulation of Polymers II, Annual Meeting of the AIChE, Pittsburgh, PA, November 2012.

"Multiscale Modeling of Polymer-Matrix Nanocomposites" (with Georgios G. Vogiatzis), 9th Hellenic Polymer Society Conference, Thessaloniki, Greece, November 2012.

"Multiscale Simulations of Macromolecular Conformation and Dynamics in Polymer Matrix Nanocomposites" (with Georgios G. Vogiatzis), international conference "Macromolecules in Constrained Environments", Les Houches, France, March 2013.

"Statistical Thermodynamics-Based Methods for the Prediction of Polymer Properties", 12$^{th}$ Joint European Thermodynamics Conference (JETC) 2013, Brescia, Italy, July 2013.

"Molecular Simulations of Polymers", 1$^{st}$ Hellenic Forum for Science, Technology and Innovation, NCSR "Demokritos", July 2013.

"Atomistic and Coarse-Grained Simulations of Polymer-Matrix Nanocomposites" (with Georgios G. Vogiatzis), CECAM Workshop on coarse-graining multicomponent soft-matter systems: Equilibrium and dynamics, Mainz, Germany, August 2013.

"Coarse-Grainining and Multiscale Simulations of Polymer-Matrix Nanocomposites" (with Georgios G. Vogiatzis and Grigorios Megariotis), Symposium on coarse-graining and multiscale modeling, Division of Physical Chemistry, 246$^{th}$ ACS National Meeting, Indianapolis, Indiana, USA, September 2013.

"Multiscale Modeling of Nanostructured Materials", QAFCO-TAMUQ Conference on Nanotechnology and Energy, Texas A&M University at Qatar, Doha, Qatar, January 2014.

"Polymeric and Nanofiller Structure and Dynamics: Hierarchical Molecular Simulations", COMPNANOCOMP Workshop, Eindhoven, The Netherlands, March 2014.

"Energy Landscape Analysis of Atomic and Polymer Glasses", Telluride Science Research Center Workshop "Searching for Reaction Coordinates and Order Parameters", Telluride, Colorado, USA, June 2014.

"Energy Landscape Analysis of Polymer Glasses" (with Nikolaos Lempesis, Georgios G. Vogiatzis, and Georgios C. Boulougouris), Eindhoven Multiscale Institute Symposium "Mechanically Driven Processes Across Scales", Eindhoven, The Netherlands, November 2014.

"Energy Landscape Analysis of Polymer Glasses" (with Nikolaos Lempesis, George G. Vogiatzis, and Georgios C. Boulougouris), 10th Hellenic Polymer Society Conference, Patras, Greece, December 2014.

"Multiscale Modeling of Polymer-Matrix Nanocomposites" (with Georgios G. Vogiatzis), KMM-VIN-FEMS Workshop "Advanced Materials Modeling for Industrial Practice", Graz, Austria, January 2015.

"Molecular Modeling of Deformation and Fracture in Polymer Networks", 16th International Conference on Deformation, Yield, and Fracture of Polymers (DYFP2015), Rolduc, Kerkrade, The Netherlands, March/April 2015.

"Multiscale Modeling of Polymer-Matrix Nanocomposites", 10th Panhellenic Scientific Conference on Chemical Engineering, Patras, Greece, June 2015.

"Molecular Simulations of Polymer-Matrix Nanocomposites", 28th European Symposium on Applied Thermodynamics (ESAT 2015), Athens, Greece, June 2015.

"Multiscale Modeling of Polymer Matrix Nanocomposites", International Workshop on Polymer Nanocomposites: Synthesis, Properties, Modeling, Applications, Athens, Greece, June 2015.

"Multiscale Simulations of Polymer Systems", IV International Young Scientists Conference, Athens, Greece, July 2015.

"Entanglements in Molecular Simulations of Polymers", Thales Workshop on Algebraic Modeling of Topological and Computational Structures, Athens, Greece, July 2015.

"Multiscale Molecular Simulations of Polymer-Matrix Nanocomposites", Workshop on Challenges in Statistical Mechanics: From Mathematics to Molecular Dynamics to Technological Applications", Imperial College London, UK, December 2015.

"Multiscale Simulations of Polymer-Matrix Nanocomposites", John M. Prausnitz Award Lecture, Conference on Properties and Phase Equilibria for Product and Process Design, Porto, Portugal, April 2016.

"Multiscale Molecular Simulations of Polymer-Matrix Nanocomposites", the 8th Global Chinese Chemical Engineers Symposium, (GCCES-8), Singapore, July 2016.

"Molecular Modeling of Materials: A Chemical Engineer's Perspective", John M. Prausnitz AIChE Institute Lecture, AIChE Annual Meeting, San Francisco, CA, USA, November 2016.

"Multiscale Simulation Approaches for Polymers at Interfaces", 3rd International Workshop on Multiscale Dynamics of Polymeric Materials organized by ESPCI Paris and Michelin, Paris, FR, November 2016.

"Multiscale Molecular Simulations of Polymer-Matrix Nanocomposites", CECAM Conference "Challenges Across Large-Scale Biomolecular and Polymer Simulations", Vienna, Austria, February 2017.

"Brownian Dynamics/Kinetic Monte Carlo Strategy for the Linear and Nonlinear Viscoelastic Properties of Polymer Melts", Mainz Materials Simulation Days 2017, CECAM-DE-SMSM Conference, Max-Planck Institut für Polymerforschung, Mainz, Germany, June 2017.

"Multiscale Molecular Simulations of Polymer-Matrix Nanocomposites", Scienomics Scimeeting and Group of Scientific Excellence meeting, NCSR "Demokritos", Athens, Greece, June 2017.

"Molecular Modeling of Materials: Promises, Challenges, and Impact" (plenary, European Materials Medal lecture), 15th Euromat Conference, Thessaloniki, Greece, September 2017.

"Molecular Modeling of Polymers: Promises, Challenges, and Impact" (DSM Life Time Achievement Award Lecture), 17th International Conference on Deformation, Yield, and Fracture of Polymers (DYFP2018), Rolduc Abbey, Kerkrade, The Netherlands, March 2018.

"Interfacial Properties of Polymer Melts: Atomistic and Mesoscopic Simulations", CECAM Workshop "Computational Biophysics on your Desktop: Is that Possible?", Trento, Italy, September 2018.

"From Chemical Constitution to the Thermal and Rheological Properties of Polymers: Algorithms for Molecular Simulations at Multiple Length and Time Scales", Symposium on "Mathematics in the Era of the 4th Industrial Revolution", National Hellenic Research Foundation, Athens, Greece, May 2019.

"Atomistic and Mesoscopic Simulations of Polymer Melts", Guggenheim Medal Lecture, Thermodynamics 2019 Conference, Punta Umbría, Spain, June 2019.

"Hybrid Particle-Field Simulations of Entangled Polymer Dynamics", International workshop on "Polymers in Fast Flows", Anacapri, Italy, July 2019.

"Atomistic and Mesoscopic Simulations of Polymer Melts", Conference "Molecular and Materials Simulation at the Turn of the Decade: Celebrating 50 Years of CECAM", Lausanne, Switzerland, September 2019.

"Multiscale Simulations of Polymers", Scientific meeting to celebrate the 50th anniversary of the Department of Physics at the University of Ioannina (by teleconference), January 2021.

"Thermodynamics of Binary Mixtures and Oligomeric Blends: A Simulation Approach Based on Kirkwood-Buff Theory" (with Stefanos D. Anogiannakis, Aikaterini A. Galata, Panagiotis C. Petris, Panagiotis Nikolaos Tzounis and Fotios Venetsanos), CECAM Flagship Workshop on Recent Progress in the Statistical Mechanics of Solutions Through Kirkwood-Buff Integrals and Related Approaches" Dijon, France (by teleconference), September 2021.

"Polymer Theory and Simulation: The First 100 Years", 13th Hellenic Polymer Society International Conference (virtual event), December 2021.

"Atomistic and Mesoscopic Modeling of Structure-Property Relations in Polymers", Plenary Talk, Vebleo Webinar on Materials Science, Engineering, and Technology, 27-30 April, 2022 (Vebleo Fellow Award).

"Meeting the Challenge of Long Time Scales in Entangled Macromolecules: From Atomistic to Mesoscopic Modeling and Simulations", Foundations of Molecular Modeling and Simulation (FOMMS) conference, Delavan, Wisconsin, July 2022 (2022 FOMMS Medal lecture).

Invited Talks at Universities and National Research Laboratories

"Molecular Modeling of Polymer Glasses", UCLA Chemical Engineering Colloquium, Los Angeles, California, October 1986.

"Interfacial Behavior of Bulk Polymers", Chemical Engineering Colloquium, University of California at Davis, November 1987.

"Structure and Thermodynamics of Liquid Polymers at Interfaces", Statistical Mechanics of Macromolecules Group seminar, University of California, San Francisco, June 1988.

"Molecular Modeling for the Prediction of Properties of Materials from Chemical Structure", Department of Chemical Engineering, University of California, San Diego, La Jolla, California, November 1988.

"Molecular Modeling Investigations of Polymers at Interfaces", Department of Polymer Science and Engineering, University of Massachusetts at Amherst, Amherst, Massachusetts, December 1988.

"Molecular Modeling for the Prediction of Properties of Materials from Chemical Structure", Department of Chemical Engineering, University of Pennsylvania, Philadelphia, Pennsylvania, December 1988.

"Molecular Modeling of Polymers at Interfaces", Chemical Engineering Seminar, California Institute of Technology, Pasadena, California, February 1989.

"Molecular Modeling of Materials", Chemical Engineering Seminar, Massachusetts Institute of Technology, Cambridge, Massachusetts, March 1989.

"Molecular Modeling of Polymers at Interfaces", Polymer Science Lecture Series, Institute of Polymer Science, The University of Akron, Akron, Ohio, January 1990.

"Molecular Modeling of Sorption and Diffusion in Zeolites", Surface Science and Catalysis Seminar, Lawrence Berkeley Laboratory, Berkeley, California, May 1990.

"Molecular Modeling of Polymers at Interfaces", Makromolekulare Chemie, Institut für Polymere, ETH-Zürich, Switzerland, June 1990.

"1. Elements of Statistical Mechanics and Introduction to Techniques for the Molecular Simulation of Materials"; "2. Molecular Simulation of Polymers: Prediction of Thermodynamic, Mechanical, Interfacial, and Rheological Properties"; "3. Molecular Simulation of Sorption and Diffusion of Small Molecular Weight Species in Zeolites and in Polymers"; National Research Centre for the Physical Sciences "Demokritos", Aghia Paraskevi, Athens, Greece, July 1990.

"Molecular Simulations of Sorption and Diffusion in Zeolites", Chemical Engineering Department, University of Florida, Gainesville, Florida, November 1990.

"Molecular Simulations of Sorption and Diffusion in Zeolites", Chemical Engineering Department, University of Houston, Houston, Texas, November 1990.

"Molecular Modeling of Polymers at Interfaces", Center for Composite Materials, University of Delaware, Newark, Delaware, December 1990.

"Molecular Modeling of Amorphous Polymers in the Bulk and at Interfaces", Chemical Engineering Colloquium, University of California, Berkeley, California, March 1991.

"Molecular Modeling of Amorphous Polymers in the Bulk and at Interfaces", Departmental Seminar, Chemical Engineering, University of Texas at Austin, Austin, Texas, October 1991.

"Molecular Modeling of Amorphous Polymers in the Bulk and at Interfaces", Institut für Thermodynamik und Reaktionstechnik, Technische Universität Berlin, Germany, May 1992.

"Molecular Simulations of Amorphous Polymers", Department of Chemistry, University of Athens, Athens, Greece, May 1992.

"Molecular Simulations of Amorphous Polymers", Department of Chemical Engineering, National Technical University of Athens, Athens, Greece, June 1992.

"Equation of State Properties of Amorphous Polymers: Monte Carlo Simulation and Mean Field Theory", Molecular Modeling Group, Institut für Polymere, ETH-Zürich, Switzerland, July 1992.

"Molecular Simulations of Amorphous Polymers", Summer School of the Physics Dept., University of Crete and Foundation for Research and Technology, Hellas, Heraklion, Crete, Greece, July 1992.

"Molecular Modeling of Sorption and Diffusion in Zeolites", Chemical Engineering Colloquium, Stanford University, Stanford, California, October 1992.

"Molecular Modeling of Polymers: Promises and Challenges", Allan P. Colburn Memorial Lecture, Department of Chemical Engineering, University of Delaware, Newark, Delaware, October 1992.

"Molecular Modeling of Adsorption and Diffusion in Zeolites", Computational Chemistry Forum, NASA Ames Research Center, Moffett Field, California, August 1993.

"Molecular Modeling of Amorphous Polymer Properties", Ernest W. Thiele Lecture, Department of Chemical Engineering, University of Notre Dame, Notre Dame, Indiana, September 1993.

"Molecular Modeling of Sorption and Diffusion in Zeolites", Competence Center for Computational Chemistry Seminar, ETH-Zürich, Switzerland, January 1994.

"Atomistic Simulations of Polymer Glasses and Melts", Sonderforschungsbereich Colloquium, Universität Ulm, Germany, January 1994.

"Atomistic Simulations of Polymer Glasses and Melts", Institut für Physik, Johannes Gutenberg-Universität, Mainz, Germany, January 1994.

"Molecular Modeling of Sorption and Diffusion in Zeolites", 1994 Robert W. Vaughan Lecture, Department of Chemical Engineering, California Institute of Technology, Pasadena, California, March 1994.

"Molecular Modeling of Sorption and Diffusion in Zeolites", Commonwealth Science and Industry Research Organisation (CSIRO), Division of Chemicals and Polymers, Clayton, Victoria, Australia, September 1994.

"Molecular Modeling of Amorphous Polymers: Promises and Challenges", Universität Leipzig, Fakultät für Physik und Geowissenschaften, Colloquium of the Sonderforschungsbereich "Molecules Interacting with Interfaces", Leipzig, Germany, January 1995.

"Molecular Simulation of Sorption and Diffusion in Zeolites: Hierarchical Approaches", Universität Leipzig, Fakultät für Physik und Geowissenschaften, Colloquium of the Sonderforschungsbereich "Molecules Interacting with Interfaces", Leipzig, Germany, January 1995.

"Atomistic Modeling of Amorphous Polymers: Promises and Challenges", Bogaziçi University, Polymer Science Centre, Istanbul, Turkey, April 1995.

"Molecular Simulations of Amorphous Polymers", Seminar, Institute of Physical Chemistry, National Center for Scientific Research "Demokritos", Athens, Greece, June 1995.

"Prediction of Material Properties with Molecular Computer Simulations: Principles and Examples of Applications", summer school short course, Institute of Physical Chemistry, National Center for Scientific Research "Demokritos", Athens, Greece, July 1995.

"Atomistic Modeling of Amorphous Polymers", Extra-colloquium, FOM Institute for Atomic and Molecular Physics, Amsterdam, The Netherlands, September 1995.

"Atomistic Modeling of Amorphous Polymers", Department of Chemistry, Rijksuniversiteit Groningen, The Netherlands, November 1995.

"Molecular Modeling of Amorphous Polymers", Technische Universiteit Eindhoven, The Netherlands, July 1996.

"Molecular Modeling as a Means for Predicting Properties of Materials", summer school short course, Institute of Physical Chemistry, National Center for Scientific Research "Demokritos", Athens, Greece, July 1996.

‘‘Simulations of Flexible Chain Molecules: From Chemical Structure to the Physical Properties of Polymers and Alkanes Sorbed in Zeolites’’, Seminar, Institute of Materials Science, National Center for Scientific Research ‘‘Demokritos’’, Athens, Greece, January 1997.

‘‘Free Energy of Polymer Melts from Atomistic Simulations’’, Seminar, Department of Chemical Engineering, University of California, Los Angeles, April 1997.

‘‘Atomistic Simulations of Chain Molecules: Some Recent Results’’, Colloquium, Department of Chemical Engineering, University of California, Berkeley, April 1997.

‘‘Atomistic Modeling of the Physical Properties of Amorphous Polymers’’, Program on Quantitative Methods in Materials Research, Institute for Theoretical Physics, University of California, Santa Barbara, April 1997.

‘‘Prediction of Sorption and Diffusion of Hydrocarbon Molecules in Zeolites’’, Program on Quantitative Methods in Materials Research, Institute for Theoretical Physics, University of California, Santa Barbara, April 1997.

‘‘Free Energy of Polymer Melts from Atomistic Simulations’’, Seminar, Department of Chemical Engineering, University of California, Santa Barbara, April 1997.

‘‘Prediction of Sorption and Diffusion of Hydrocarbons in Zeolites through New, Hierarchical Molecular Simulation Techniques’’, Group Seminar of Professor Horia Metiu, Department of Chemistry, University of California, Santa Barbara, April 1997.

‘‘From Chemical Structure to the Physical Properties of Materials: What can Molecular Simulations Contribute?’’, Seminar, Department of Chemical Engineering, University of Patras and Institute for Chemical Engineering and High Temperature Chemical Processes, Patras, Greece, May 1997.

‘‘From Chemical Structure to the Physical Properties of Materials: What can Molecular Simulations Contribute?’’, Seminar, Institute of Physical Chemistry, National Center for Scientific Research ‘‘Demokritos’’, Athens, Greece, May 1997.

‘‘Atomistic Modeling of Polymers: Elasticity, Viscosity, and Fluid-Phase Equilibria’’, Seminar, Department of Materials Science and Engineering, Pennsylvania State University, University Park, PA, USA, February 1998.

‘‘Hierarchical Modeling Strategies for Polymers: Elasticity, Viscosity, and Fluid-Phase Equilibria’’, Materials Modeling Laboratory Seminar, Department of Materials, Oxford University, UK, March 1998.

‘‘Molecular Simulations of Polymer Systems: Elasticity, Viscosity, and Phase Equilibria’’, Colloquium, Physics Department, University of Crete, Heraklion, Greece, May 1998.

‘‘Efficient Monte Carlo Strategies for the Equilibration of Atomistic Models of Chain Fluids’’, Royal Australian Chemical Institute Polymer Seminar, Commonwealth Science and Industry Research Organisation (CSIRO), Clayton, Victoria, Australia, July 1998.

‘‘Efficient Monte Carlo Strategies for the Equilibration of Atomistic Models of Chain Fluids’’, Seminar, Research School of Chemistry, Australian National University, Canberra, Australia, July 1998.

‘‘Efficient Simulation Strategies for the Equilibration of Atomistic Models of Chain Fluids’’, Seminar, Sydney University Polymer Center, Sydney, Australia, July 1998.

‘‘Diffusion of Gases in Polymers: From the Molecular to the Macroscopic Level’’, Symposium on Topics in Mass Transfer in Honor of R.M. Barrer and his School, Institute of Physical Chemistry, NCSR ‘‘Demokritos’’, Athens, Greece, October 1998.

‘‘Research in Our Country: Questions to Ponder’’, Round Table organized by the University of Patras and coordinated by the General Secretary of Research and Technology of Greece, March 1999.

‘‘Molecular Modeling of Polymers: Elasticity, Viscosity, and Fluid-Phase Equilibria’’, Colloquium, Center for Nonlinear Systems and Complex Phenomena, Université Libre de Bruxelles, Belgium, March 1999.

‘‘From Chemical Structure to the Physical Properties of Polymer Systems: What can Molecular Simulations Offer?’’, seminar, Department of Mechanical and Industrial Engineering, University of Thessaly, Volos, Greece, April 1999.

‘‘Prediction of Structure-Property Relations in Materials With Computational Techniques’’, seminar, Graduate Programme on Processes and Technology of Advanced Materials, Aristotelian University of Thessaloniki, Greece, June 1999.

‘‘Hierarchical Methods for Modeling Molecular Motion and Deformation in Polymers’’, seminar, Recent Advances on Polymer Science and Technology Seminar Series, Cátedra Repsol, Escuela Técnica Superior de Ingenieros Industriales, Universidad Politécnica de Madrid, March 2000.

‘‘Computer Simulations of Materials: Structure-Property Relations’’, ‘‘Epistemes Koinonia’’ lecture series, National Hellenic Research Foundation, April 2000.

‘‘Computer Simulation of High Polymers: Meeting the Challenge of Long Time Scales’’, seminar, Department of Physics, Technical University of Twente, Enschede, The Netherlands, October 2001.

‘‘Computer Simulations of Sorption and Transport in Zeolites’’, Heyrovský Institute of Physical Chemistry, Academy of Sciences of the Czech Republic, Prague, June 2002.

“Structure-Property Relations in Polymers Through New Computational Methods”, seminar, Centre for Research and Technology, Hellas (CERTH), Thessaloniki, Greece, February 2003.

“Computational Materials Science”, 2-hour lecture, the Summer School of the Physical Chemistry Institute, NCSR “Demokritos”, July 2003.

“Mathematical Analysis and Computer Simulation in Materials Science and Engineering”, Seminar presented to the interdepartmental program of graduate studies “Mathematical Modeling in Modern Technologies and in Economics”, National Technical University of Athens, December 2004.

“Hierarchical Simulations of Polymeric Materials”, Department of Chemistry Seminar, National and Kapodistrian University of Athens, January 2005.

“Hierarchical Modeling of Polymeric Materials”, University of Vienna, Physics Department, June 2006.

“Computer Simulations of Polymeric Materials”, Summer School of the National Center for Scientific Research “Demokritos”, July 2006.

“Multiscale Modeling of Materials”, Kolloquium, Fakultät für Physik und Geowissenschaften und Fakultät für Chemie und Mineralogie, Universität Leipzig, Germany, October 2006.

“Hierarchical Modeling of Polymeric Materials”, Theoretical Physics Group (Prof. Dr. Erwin Frey), Ludwig-Maximilians-Universität, München, Germany, February 2007.

“Hierarchical Simulations of Polymeric Materials”, Solid State Colloquium, Fosrchungszentrum Jülich, Germany, November 2007.

“Computer Simulation of Polymeric Materials: Meeting the Challenge of Long Time Scales”, seminar, Department of Materials Science and Technology, University of Crete, November 2007.

“From Chemical Structure to Physical Properties of Polymeric Systems via Multiscale Modeling”, Chemical Engineering Centenary Seminar Series, Imperial College London, February 2008.

"Molecular Simulations of Amorphous Polymers: Meeting the Challenge of Long Time Scales", Colloquium, Eduard-Zintl-Institut für Anorganische und Physikalische Chemie, Technische Universität Darmstadt, Germany, March 2008.

"Multiscale Simulations of Amorphous Polymers: Meeting the Challenge of Long Time Scales", departmental seminar, Department of Chemical Engineering, University of Texas at Austin, Austin, TX, USA, November 2008.

"Hierarchical Simulations of Polymers: Meeting the Challenge of Long Time Scales", Process and Energy Laboratory, Delft University of Technology, Delft, The Netherlands, January 2010.

"Multiscale Simulations of Amorphous Polymers: Meeting the Challenge of Long Time Scales", Department of Chemical Engineering, University of Manchester, Manchester, UK, April 2010.

"Progress and Outlook in Monte Carlo Simulations", CSIRO Materials Science and Engineering, Clayton, Victoria, Australia, November 2010.

"Computational Prediction of the Physical Properties of Polymer Melts: Overcoming the Challenge of Long Time Scales", CSIRO Materials Science and Engineering, Clayton, Victoria, Australia, November 2010.

"Glasses: A Grand Challenge for Molecular Simulation", CSIRO Materials Science and Engineering, Clayton, Victoria, Australia, November 2010.

"Computational Materials Science: From Molecular Structure to Macroscopic Properties", Summer School of the National Center for Scientific Research "Demokritos", Athens, Greece, July 2012.

"Molecular Simulations of Polymers: Melts, Networks, Nanocomposites", Bird-Stewart-Lightfoot Lecture, Department of Chemical Engineering, University of Wisconsin, Madison, May 2013.

"Molecular Simulations of Polymers", Seminar, Department of Chemical Engineering, Massachusetts Institute of Technology, May 2013.

"Multiscale Modeling of Polymer-Matrix Nanocomposites", Oryx GTL Excellence in Chemical Engineering Seminar, Texas A&M University at Qatar, Doha, Qatar, March 2015.

"Multiscale Simulations of Polymer-Matrix Nanocomposites", PRISM/PCCM Seminar, Princeton University, October 2015.

"Multiscale Simulations of Polymer Systems", School of Applied Mathematics and Physical Sciences, NTU Athens, October 2015.

"Atomistic and Mesoscopic Simulations of Polymer Melts", "Alkiviades Ch. Payatakes" Distinguished Lecture, FORTH/ICE-HT, Patras, Greece, December 2018.

"Atomistic and Mesoscopic Modeling of Structure-Property Relations in Polymers", Seminar, Department of Chemical and Petroleum Engineering, University of Pittsburgh, PA, USA (via teleconference), March 2021.

"Multiscale Simulations of Polymers", Seminar, Department of Chemical Engineering, University of Patras, Greece (via teleconference), March 2021.

“Atomistic and Mesoscopic Simulations of Polymeric Materials”, Seminar, Institute of Electronic Structure and Laser, Foundation of Research and Technology, Hellas (IESL-FORTH) (by teleconference), May 2021.

“Atomistic and Mesoscopic Simulations of Polymeric Materials”, seminar presented to the interdepartmental program of graduate studies “Mathematical Modeling in Modern Technologies and in Financial Engineering”, National Technical University of Athens, April 2022.

“Atomistic and Mesoscopic Modeling of Structure-Property Relations in Polymers”, ATOMS-Seminar, Research Group of Prof. Frederico Wanderley Tavares, Federal University of Rio de Janeiro, Brazil, September 2022.

Invited Talks at Industrial Research Centers

"Molecular Simulation of Glassy Amorphous Polymers: From Chemical Structure to Mechanical Properties", E.I. du Pont de Nemours Experimental Station, Central Research and Development, Polymer Physics Group, Wilmington, Delaware, January 1987.

"Molecular Modeling of Polymer Glasses", IBM Almaden Research Center, Polymer Science and Technology Research Division, June 1987.

"Structure and Thermodynamics of Bulk Polymers at Interfaces", E.I. Du Pont de Nemours Experimental Station, Polymer Products Department, Polymer Scouting Group, Wilmington, Delaware, November 1987.

"Interfacial Structure and Thermodynamics of Polymer Melts", IBM Almaden Research Center, Surface and Interface Dynamics Research Division, December 1987.

"Molecular Modeling for the Prediction of Properties of Materials from Chemical Structure", The BFGoodrich Company Research and Development Center, Brecksville, Ohio, June 1988.

"Molecular Modeling for the Prediction of Properties of Materials from Chemical Structure", E.I. Du Pont de Nemours Experimental Station, Central Research and Development, Wilmington, Delaware, August 1988.

"Prediction of Sorption and Diffusion in Zeolite Catalysts", W.R.Grace & Co., Washington Research Center, Columbia, Maryland, August 1988.

"Prediction of Properties of Materials Through Molecular Modeling", The Dow Chemical Company, M.E. Pruitt Research Center, Midland, Michigan, October 1988.

"Computer Simulation of Sorption and Diffusion in Zeolites", Engineering and Technology Services Division, Research and Development Department, Technical Center, Union Carbide Corporation, South Charleston, West Virginia, March 1989.

"Surface and Interfacial Properties of Polymers: A Molecular Modeling Approach", Process Technologies Laboratory, 3M Corporate Research, 3M Center, St.Paul, Minnesota, May 1989.

"Molecular Modeling of Materials", seminar, Air Products and Chemicals, Inc., Allentown, Pennsylvania, May 1989.

"An Overview of Applied Statistical Mechanics, Molecular Simulation Methods, and Their Application to the Study of Sorption and Diffusion in Zeolites", tutorial, W.R.Grace & Co., Washington Research Center, Columbia, Maryland, January 1990.

"Molecular Modeling of Sorption and Diffusion in Zeolites", UOP/Allied Signal Invitational Lecture Series, UOP Research Center and Allied-Signal Engineering Materials Research Center, Des Plaines, Illinois, October 1990.

"Molecular Simulations of Sorption and Diffusion in Zeolites", W.R. Grace & Co. Washington Research Center, Columbia, Maryland, March 1991.

"Predictions of the Equation of State Behavior or Amorphous Polymers and of Sorption and Diffusion of Gases in them through Molecular Simulation", B.F. Goodrich Corporate Research Center, Brecksville, Ohio, March 1991.

"Molecular Modeling of Amorphous Polymers in the Bulk and at Interfaces", BIOSYM Technologies, Inc., San Diego, California, May 1991.

"Molecular Simulations of Sorption and Diffusion in Zeolites", Mobil Research and Development Corporation, Paulsboro Research Laboratory, Paulsboro, New Jersey, June 1991.

"Molecular Modeling of Amorphous Polymers", BP International Ltd., Sunbury Research Center, Sunbury-on-Thames, England, September 1992.

‘‘Molecular Modeling of Polymer Physical Properties’’, DSM Research, Geleen, The Netherlands, October 1998.

‘‘Computational Materials Science: Status and Perspectives’’, BP Research Center, Naperville, Illinois, USA, November 2000.

‘‘Novel Monte Carlo Methods and Algorithms for Predicting Phase Equilibria’’, Molecular Simulations, Inc., San Diego, California, USA, November 2000.

‘‘Structure and Dynamics of Polymers at Interfaces’’, DSM Research, Geleen, The Netherlands, February 2002.

“Hierarchical Modeling of Polymer Properties”, DSM Research, Geleen, The Netherlands, September 2006.

“Molecular Modeling of Cavitation in Polymer Networks”, DSM Research, The Netherlands, June 2010.

“Hierarchical Modeling of the Physical Properties of Polymers”, Mitsui Chemical Company, Sodegaura, Japan, September 2011.

“Hierarchical Modeling of Nanostructured Materials”, DSM Research, Geleen, The Netherlands, September 2016.

“Molecular Modeling of Materials: Promises, Challenges, and Impact”, Extra Brightlands Science Lecture, Brightlands Chemelot Campus, Geleen, The Netherlands, March 2018.

“Hybrid Particle-Field Simulations of Entangled Polymer Dynamics”, DSM Research, Geleen, The Netherlands, September 2019.

“Atomistic and Mesoscopic Modeling for Polymer Properties”, Braskem Innovation and Technology Team (via teleconference), October 2020.

“Mesoscopic Modeling of Self-Assembling Soft-Matter Systems”, Solvay S.A. (via teleconference), May 2021.

“Atomistic and Mesoscopic Modeling of Structure-Property Relations in Polymers”, Materials Design Webinar, April 2022.

Contributed Papers (speaker is underlined)

Theodorou, D.N. "A Model for Chain Orientation and Local Properties at a Bulk Polymer/Solid Interface"; Composites portion of the AIChE Conference on Emerging Technologies in Materials, Minneapolis, Minnesota, August 1987.

Theodorou, D.N. "Molecular Modeling for the Prediction of Properties of Materials from Chemical Structure"; 1987 Annual Meeting of the American Institute of Chemical Engineers, New York, N.Y., November 1987.

Theodorou, D.N. "A Lattice Model for Structure and Thermodynamic Properties of Bulk Polymer/Solid and Bulk Polymer/Gas Interfaces"; 1987 Annual Meeting of the American Institute of Chemical Engineers, New York, N.Y., November 1987.

June, R.L.; Bell, A.T.; Theodorou, D.N. "Sorption and Transport of Hydrocarbons in Pentasil Zeolites: A Molecular Modeling Approach"; 196th National Meeting of the American Chemical Society, Los Angeles, California, September 1988.

Mansfield, K.F.; Theodorou, D.N. "Atomistic Simulation of Glassy Polymer Surfaces"; 1988 Pacific Conference on Chemistry and Spectroscopy, San Francisco, California, October 1988.

June, R.L.; Bell, A.T.; Theodorou, D.N. "Computer Simulation of Transport and Sorption in Zeolitic Systems"; 1988 Pacific Conference on Chemistry and Spectroscopy, San Francisco, California, October 1988.

Mansfield, K.F.; Theodorou, D.N. "Atomistic Simulation of Glassy Polymer Surfaces and Glassy Polymer/Solid Interfaces"; 1988 Annual Meeting of the American Institute of Chemical Engineers, Washington, D.C., November 1988.

Mansfield, K.F.; Theodorou, D.N. "Interfacial Dynamics of Macromolecular Systems: A Monte Carlo Simulation Approach"; 1988 Annual Meeting of the American Institute of Chemical Engineers, Washington, D.C, December 1988.

June, R.L.; Bell, A.T.; Theodorou, D.N. "Atomistic Modeling of Sorption and Transport in Pentasil Zeolites"; 1988 Annual Meeting of the American Institute of Chemical Engineers, Washington, D.C., December 1988.

Mansfield, K.F.; Theodorou, D. "Molecular Simulation of Glassy Polymer/Graphite Interfaces"; 1989 Annual Meeting of the American Institute of Chemical Engineers, San Francisco, CA, November 1989.

Theodorou, D.N. "Molecular Modeling of Structure and Thermodynamic Properties of Polymers at Interfaces", 33rd IUPAC Symposium on Macromolecules, Montréal, Quebec, Canada, July 1990.

Dodd, L.R.; Theodorou, D.N. "PVT Properties of Polymer Liquids from Detailed Chain Geometry and Energetics", Symposium on Models for Polymer Thermodynamics, Annual Meeting of the American Institute of Chemical Engineers, Chicago, Illinois, November 1990.

Mansfield, K.F.; Theodorou, D.N. "Atomistic Molecular Dynamics Simulation of a Polymer/Vacuum Interface", Symposium on Polymer Surfaces and Interfaces, Annual Meeting of the American Institute of Chemical Engineers, Chicago, Illinois, November 1990.

Boone, T.D.; Theodorou, D.N. "Structure and Thermodynamics of Bulk Glassy Polymers Through Monte Carlo Simulations", Annual Meeting of the American Institute of Chemical Engineers, Chicago, Illinois, November 1990.

Snurr, R.Q.; June, R.L.; Bell, A.T.; Theodorou, D.N. "Molecular Simulations of Methane in Silicalite", Annual Meeting of the American Institute of Chemical Engineers, Chicago, Illinois, November 1990.

June, R.L.; Theodorou, D.N. "Molecular Dynamics Simulations of Sorbate Molecules in Zeolites", Annual Meeting of the American Institute of Chemical Engineers, Chicago, Illinois, November 1990.

Dodd, L.R.; Theodorou, D.N. "Theory and Simulation of Polymer Melts in the Bulk and at Free Surfaces", Annual Meeting of the American Institute of Chemical Engineers, Los Angeles, California, November 1991.

Sevick, E.M.; Bell, A.T.; Theodorou, D.N. "Diffusion of Flexible Penetrants in Geometrically Confined Pores: Transition State Theory Applied to Alkane Diffusion in Zeolites", Annual Meeting of the American Institute of Chemical Engineers, Los Angeles, California, November 1991.

Cook, S.J.; Chakraborty, A.K.; Bell, A.T.; Theodorou, D.N. "Structure and Electronic Properties of the Acid Site in H-ZSM-5", 203rd National Meeting of the American Chemical Society, San Francisco, California, April 1992.

Sevick, E.M.; Bell, A.T.; Theodorou, D.N. "Transition State Theory Applied to Alkane Diffusion in Zeolites", 203rd National Meeting of the American Chemical Society, San Francisco, California, April 1992.

Snurr, R.Q.; Bell, A.T.; Theodorou, D.N. "Molecular Simulations of the Adsorption of Aromatics in Silicalite", Annual Meeting of the American Institute of Chemical Engineers, Miami, Florida, November 1992.

Maginn, E.; Bell, A.T.; Theodorou, D.N. "Prediction of the Transport Diffusivity of Methane in Silicalite Using Equilibrium and Non-equilibrium Simulation Techniques", Annual Meeting of the American Institute of Chemical Engineers, Miami, Florida, November 1992.

Boone, T.D.; Theodorou, D.N. "Monte Carlo Simulations of Bulk Vinyl Polymers in the Glass and Melt for Penetrant Sorption Predictions", Annual Meeting of the American Institute of Chemical Engineers, Miami, Florida, November 1992.

Greenfield, M.L.; Theodorou, D.N. "Geometric Analysis of Diffusion Paths in Glassy Polymers", Annual Meeting of the American Institute of Chemical Engineers, Miami, Florida, November 1992.

Cook, S.J., Theodorou, D.N., Chakraborty, A.K., Bell, A.T. "Structure and Electronic Properties of the Acid Site in H-ZSM-5", Annual Meeting of the American Institute of Chemical Engineers, Miami, Florida, November 1992.

Bell, A.T.; Chakraborty, A.K.; Theodorou, D.N. "Theoretical Predictions of the Properties of Zeolite Catalysts", Annual Meeting of the American Institute of Chemical Engineers, Miami, Florida, November 1992.

Pant, P.V.K.; Theodorou, D.N. "A Novel Monte Carlo Scheme for the Simulation of Polymer Melts in the Bulk and at Interfaces", Annual Meeting of the American Institute of Chemical Engineers, St. Louis, Missouri, November 1993.

Snurr, R.Q.; Bell, A.T.; Theodorou, D.N. "Simulation Strategies for the Study of Adsorption and Diffusion of Aromatics in Silicalite", Annual Meeting of the American Institute of Chemical Engineers, St. Louis, Missouri, November 1993.

Theodorou, D.N. "Prediction of the Properties of Amorphous Polymers through Molecular Simulation", 3rd Panhellenic Conference on Polymers, Aristotle University of Thessaloniki, Thessaloniki, Greece, December 1993.

Pant, P.V.K.; Theodorou, D.N. "Simulations of the Structure and Thermophysical Properties of Polydisperse Polymer Melts", Annual Meeting of the American Institute of Chemical Engineers, San Francisco, California, November 1994.

Greenfield, M.L.; Theodorou, D.N. "Molecular-Level Description of Methane Diffusion in Glassy Atactic Polypropylene Using Multidimensional Transition-State Theory", Annual Meeting of the American Institute of Chemical Engineers, San Francisco, California, November 1994.

Kyrlidis, A.; Chakraborty, A.K.; Bell, A.T.; Theodorou, D.N. "Electronic Structure Calculations of Adsorption in H-ZSM5 Zeolites", Annual Meeting of the American Institute of Chemical Engineers, San Francisco, California, November 1994.

Fischel, L.B.; Theodorou, D.N. "Self-Consistent Field Model of the Polymer/Diblock Copolymer/Polymer Interface", Annual Meeting of the American Institute of Chemical Engineers, Miami, Florida, November 1995.

Fischel, L.B.; Theodorou, D.N. "Modeling Structure and Adhesion at Polymer/Copolymer/Polymer Interfaces", 5th European Symposium on Polymer Blends, Maastricht, The Netherlands, May 1996.

Mavrantzas, V.G.; Theodorou, D.N. "From Chain Chemical Structure to Polymer Melt Elasticity: The Implementation of New Monte Carlo Techniques" (poster presentation), 6th European Polymer Federation Symposium on Polymeric Materials, Aghia Pelaghia, Crete, Greece, October 1996.

Spyriouni, D., Economou, I.G.; Theodorou, D.N. "Phase Equilibria of Polymer Systems from Molecular Simulation: Test of the Chain Increment Method for Estimation of Chemical Potentials" (poster presentation), 6th European Polymer Federation Symposium on Polymeric Materials, Aghia Pelaghia, Crete, Greece, October 1996.

Kopsias, N.; Theodorou, D.N. "Computer Simulation of the Structure and Thermodynamic Properties of Glasses" (poster presentation), 6th European Polymer Federation Symposium on Polymeric Materials, Aghia Pelaghia, Crete, Greece, October 1996.

Samara, C.T.; Antoniadis, S.; Theodorou, D.N. "Development of a Reliable Molecular Model for Polypropylene" (poster presentation), 6th European Polymer Federation Symposium on Polymeric Materials, Aghia Pelaghia, Crete, Greece, October 1996.

Chassapis, C.S.; Petrou, J.K.; Petropoulos, J.H.; Theodorou, D.N. "Analysis of Computed Trajectories of Penetrant Micromolecules in a Simulated Polymeric Material" (poster presentation), 6th European Polymer Federation Symposium on Polymeric Materials, Aghia Pelaghia, Crete, October 1996.

Mavrantzas, V.G.; Theodorou, D.N. ''From Chain Chemical Constitution to Melt Elasticity: An Application of New, Fast Monte Carlo Algorithms'', Symposium on Molecular Modeling of Polymers, 213th ACS National Meeting, San Francisco, California, April 1997.

Theodorou, D.N. ''From Microscopic Structure to the Separation Properties of Polymeric and Microporous Materials: What can Molecular Simulations Contribute?'', 1st Panhellenic Scientific Meeting of Chemical Engineers, Patras, Greece, May 1997.

Mavrantzas, V. G.; Theodorou, D. N. ''From Chemical Structure to the Viscoelasticity of Polymer Melts: Application of a New, Hierarchical Molecular Simulation Method'', 1st Panhellenic Scientific Meeting of Chemical Engineers, Patras, Greece, May 1997.

Spyriouni, T.; Economou, I. G.; Theodorou, D. N. ''Thermodynamics of Chain Fluids from Atomistic Simulation: A Test of the Chain Increment Method for Chemical Potential'', 1st Panhellenic Scientific Meeting of Chemical Engineers, Patras, Greece, May 1997.

Boulougouris, G.; Economou, I. G.; Theodorou, D. N. ''Molecular Simulation of Thermodynamic Properties and Phase Equilibria of Water'', 1st Panhellenic Scientific Meeting of Chemical Engineers, Patras, Greece, May 1997.

Kopsias, N. P.; Theodorou, D. N. ''Prediction of Structural Relaxation Phenomena in Amorphous Materials Using Transition-State Theory'' (poster presentation), 3rd International Discussion Meeting on Relaxations in Complex Systems, Vigo, Spain, June 1997.

Harmandaris, V.A., Mavrantzas, V.G.; Theodorou, D.N. ''From the Chemical Structure to the Rheological Properties of Polymer Melts: Implementation of a New, Hierarchical Molecular Simulation Method'', 4th Panhellenic Conference on Polymers, Patras, Greece, November 1997.

Samara, C.T.; Antoniadis, S.; Theodorou, D.N. ''Development of a Reliable Molecular Model for Polypropylene'', 4th Panhellenic Conference on Polymers, Patras, Greece, November 1997.

Spyriouni, T.; Economou, I.G.; Theodorou, D.N. ''Phase Equilibria of Macromolecular Systems Via Computer Simulation''(poster presentation), 4th Panhellenic Conference on Polymers, Patras, Greece, November 1997.

Kopsias, N. P.; Theodorou, D.N. ''Molecular Simulation of Structural Relaxation Phenomena in Amorphous Materials Using Transition-State Theory'' (poster presentation), 4th Panhellenic Conference on Polymers, Patras, Greece, November 1997.

Spyriouni, T.; Economou, I.G.; Theodorou, D.N. ''Simulations of Macromolecular Systems as a Tool for the Design of Chemical Processes and Products'', 2nd Panhellenic Symposium on Chemical Research and Industry, NCSR ''Democritos'', Athens, Greece, December 1997.

Mavrantzas, V.G.; Harmandaris, E.A.; Theodorou, D.N. ''Atomistic Simulation of the Viscoelasticity of Linear Polyethylene Melts'', 1st Hellenic Society of Rheology Meeting, Heraklion, Crete, Greece, August 1998.

Greenfield, M.L.; Theodorou, D.N. ‘‘Coarse-Grained Simulation Method for Predicting Penetrant Diffusivity in a Glassy Polymer from Molecule Jump Rates’’, Annual Meeting of the American Institute of Chemical Engineers, Miami, Florida, November 1998.

Harmandaris, V. A.; Mavrantzas, V.G.; Theodorou, D.N. ‘‘Atomistic Simulation of the Stress Relaxation Modulus of Polyethylene Melts After Cessation of Uniaxial Extensional Flow’’, 2nd Panhellenic Scientific Meeting of Chemical Engineers, Thessaloniki, Greece, May 1999.

Gergidis, L.N.; Theodorou, D.N. ‘‘Investigation of the Dynamics of n-Butane – Methane Mixtures in Zeolites Using Atomistic Molecular Dynamics Simulations’’, 2nd Panhellenic Scientific Meeting of Chemical Engineers, Thessaloniki, Greece, May 1999.

Zervopoulou, E.; Mavrantzas, V.G.; Theodorou, D.N. ‘‘Atomistic Simulation of High-Molecular Weight Polyethylene Melts and of the Solubility of Small Alkanes Therein’’, 2nd Panhellenic Scientific Meeting of Chemical Engineers, Thessaloniki, Greece, May 1999.

Kopsias, N.P.; Theodorou, D.N. ‘‘Molecular Simulation of Structural Relaxation Phenomena in Amorphous Materials Using Transition-State Theory’’, 2nd Panhellenic Scientific Meeting of Chemical Engineers, Thessaloniki, Greece, May 1999.

Terzis, A.F.; Theodorou, D.N. ‘‘Coarse-Grained Molecular Model of Polypropylene – Polyamide 6 Interfaces’’, 2nd Panhellenic Scientific Meeting of Chemical Engineers, Thessaloniki, Greece, May 1999.

Karayiannis, N.C.; Theodorou, D.N. ‘‘A Study of Diffusion in Disordered Media: Effects of Temporal and Spatial Heterogeneity’’, 2nd Panhellenic Scientific Meeting of Chemical Engineers, Thessaloniki, Greece, May 1999.

Theodorou, D.N.; Doxastakis, M.; Samara, C.; Antoniadis, S.J.; and Fytas, G. ‘‘Segmental Dynamics in Polymer Melts and Blends: Molecular Simulations Confronted With Experimental Measurements’’, Annual Meeting of the American Institute of Chemical Engineers, Los Angeles, California, Nov. 2000.

Terzis, A.F.; Theodorou, D.N.; Stroeks, A.A.M. ‘‘Hierarchical Modeling of Structure and Adhesion at Polymer/Polymer Interfaces Strengthened With Copolymers’’, Annual Meeting of the American Institute of Chemical Engineers, Los Angeles, California, November 2000.

Theodorou, D.N.; Economou, I.G.; Boulougouris, G.C. ‘‘Monte Carlo Simulation of Aqueous Systems Using Novel Simulation Methodologies’’, Annual Meeting of the American Institute of Chemical Engineers, Los Angeles, California, November 2000.

Theodorou, D.N.; Gergidis, L.N.; Jobic, H. ‘‘Molecular Dynamics Simulation and Quasielastic Neutron Scattering Investigation of Methane – n-Butane Mixtures in Silicalite’’, Annual Meeting of the American Institute of Chemical Engineers, Los Angeles, California, November 2000.

Theodorou, D.N.; Mavrantzas, V.G.; Zervopoulou, E.; Doxastakis, M. ‘‘Prediction of Physical Properties of Polymer Melts Through New, Connectivity-Altering Monte Carlo Algorithms’’, Annual Meeting of the American Institute of Chemical Engineers, Los Angeles, California, November 2000.

Theodorou, D.N.; Mavrantzas, V.G.; Harmandaris, V. ‘‘Rheological Properties of Polymer Melts from Molecular Constitution Through a Hierarchical Modeling Approach’’, Annual Meeting of the American Institute of Chemical Engineers, Los Angeles, California, November 2000.

Theodorou, D.N.; Mavrantzas, V.G.; Karayiannis, N.Ch. ‘‘Effects of Jump Rate Distribution and Spatial Heterogeneity on Diffusion in Disordered Media’’, (poster presentation), Annual Meeting of the American Institute of Chemical Engineers, Los Angeles, California, November 2000.

Peristeras, L.D.; Economou, I.G.; Theodorou, D.N. “Elementary Moves in Monte Carlo Simulation of Linear and Branched Polyolefins” (poster presentation), 19th European Seminar on Applied Thermodynamics, Santorini, Greece, September 2002.

Raptis, V.E.; Melissas, V.S.; Economou, I.E.; Theodorou, D.N.; Sanopoulou, M.; Petrou, J.; Petropoulos, J.H. “Development of Novel Polymeric Membranes for Natural Gas Hydrocarbon Separation Through Experimental Measurements, Quantum Mechanics, Molecular Simulation and Macroscopic Modeling” (poster presentation), 19th European Seminar on Applied Thermodynamics, Santorini, Greece, September 2002.

Tsolou, G.; Mavrantzas, V.G.; Theodorou, D.N. “Atomistic Molecular Dynamics Simulation of Polydisperse *cis*-1,4 polybutadiene Melts”, 4th Panhellenic Scientific Conference in Chemical Engineering, Patras, Greece, May 2003.

Margaritis, N.A.; Vergadou, N.; Zacharopoulos, N.; Theodorou, D.N. “Coarse-Graining Methodology for the Simulation of Structure of Stiff-Chain Polymers”, 4th Panhellenic Scientific Conference in Chemical Engineering, Patras, Greece, May 2003.

Raptis, B.; Economou, I.G.; Petrou, J.; Petropoulos, J.H.; Theodorou, D.N. “Modeling the Molecular Structure and Macroscopic Transport Properties of New Polymeric Membranes Through Molecular Simulation”, 4th Panhellenic Scientific Conference in Chemical Engineering, Patras, Greece, May 2003.

Vergadou, N.; Theodorou, D.N. “Determination of Diffusion Paths in Glassy Polymers Using Multidimensional Transition-State Theory”, 19th Panhellenic Conference on Solid-State Physics and Materials Science, Thessaloniki, Greece, September 2003.

Logotheti, E.G.; Theodorou, D.N. “Computational Prediction of Polypropylene Melt Properties”, 5th Panhellenic Scientific Conference in Chemical Engineering, Thessaloniki, Greece, May 2005.

Tzoumanekas, Ch.; Theodorou, D.N. “Topological Analysis of Entanglements in Polymer Melts”, 5th Panhellenic Scientific Conference in Chemical Engineering, Thessaloniki, Greece, May 2005.

Daoulas, K.; Theodorou, D.N.; Roos, A.; Creton, A. “Prediction of Properties of Self-Adhesive Materials Based on Styrenic Block Copolymers with Self-Consistent Field Methods”, 5th Panhellenic Scientific Conference in Chemical Engineering, Thessaloniki, Greece, May 2005.

Tzoumanekas, Ch.; Theodorou, D.N. “Entanglements and Underlying Topology in Polymer Melts”, Annual AIChE meeting, San Francisco, USA, November 2006.

Uhlherr, A.; Theodorou, D.N. “Accelerating Molecular Simulations by Reversible Mapping Between Local Minima”, Annual AIChE meeting, San Francisco, USA, November 2006.

Tsalikis, D.; Boulougouris, G.C.; Peristeras, L.; Theodorou, D.N. "Plastic Deformation in Amorphous Polymers: A Free Energy Landscape Approach", Annual AIChE meeting, San Francisco, USA, November 2006.

Tzoumanekas, Ch.; Anogiannakis, S.D.; Theodorou, D.N. "Atomistic Chains and Primitive Paths in Entangled Polymer Melts: Chain Size and Shape Dependence of the Tendency for Entanglement", 4th Annual European Rheology Conference (AERC 2007), Napoli, Italy, April 2007.

Boulougouris, G.C.; Tsalikis, D.; Peristeras, L.; Theodorou, D.N. "Atomistic Simulations of Polymeric Glasses Over a Wide Time Scale", poster presentation, 11th International Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD 2007), Hersonissos, Crete, Greece, May 2007.

Kamio, K.; Moorthi, K.; Theodorou, D.N. "Simulation of Atomistic and Coarse-Grained Poly(ethylene terephthalate)", poster presentation, 11th International Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD 2007), Hersonissos, Crete, Greece, May 2007.

Johansson, E.; Bolton, K.; Ahlström, P. "Molecular Simulation of Solubilities and Structure of Water in n-Alkanes and Polyethylene", poster presentation, 11th International Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD 2007), Hersonissos, Crete, Greece, May 2007.

Vergadou, N.; Theodorou, D.N. "Computational Study of Permeability of Glassy Polymers to Gases", poster presentation, 11th International Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD 2007), Hersonissos, Crete, Greece, May 2007.

Tzoumanekas, Ch.; Theodorou, D.N. "Entanglement Molecular Weight and Topological Constraints in Polymer Melts", poster presentation, 11th International Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD 2007), Hersonissos, Crete, Greece, May 2007.

Logotheti, G.-E.; Theodorou, D.N. "Segmental and Chain Dynamics of Isotactic Polypropylene Melts", poster presentation, 11th International Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD 2007), Hersonissos, Crete, Greece, May 2007.

Spyriouni, T.; Tzoumanekas, Ch.; Theodorou, D.N. "Coarse-Grained and Reverse-Mapped United-Atom Simulations of Long-Chain Atactic Polystyrene Melts: Structure, Thermodynamic Properties, Chain Conformation, and Entanglements", poster presentation, 11th International Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD 2007), Hersonissos, Crete, Greece, May 2007.

Vergadou, B.; Theodorou, D.N. "Molecular Simulation for the Prediction of Permeability of Glassy Polymers by Gases", 6th Panhellenic Scientific Conference in Chemical Engineering, Athens, Greece, May-June 2007.

Tsalikis, D.; Peristeras, L. ; Boulougouris, G.C.; Theodorou, D.N. "Computational Study of the Dynamical Properties of Glassy Polymers Using the Picture of Inherent Structures", 6th Panhellenic Scientific Conference in Chemical Engineering, Athens, Greece, May-June 2007.

Tsalikis, D.; Peristeras, L. ; Boulougouris, G.C.; Theodorou, D.N. "Parallel Programming Strategies in the Computation of Saddle Points on Multidimensional Potential Energy Surfaces", 6th Panhellenic Scientific Conference in Chemical Engineering, Athens, Greece, May-June 2007.

Papadopoulos, G.; Theodorou, D.N. "Mesoscopic Simulations of the Diffusivity of Ethane in Beds of NaX Zeolite Crystals: Comparison With Pulsed Field Gradient NMR Measurements", 6th Panhellenic Scientific Conference in Chemical Engineering, Athens, Greece, May-June 2007.

Theodorou, D.N. "Accomplishments of Computational Materials Science and Engineering", Symposium "NTU in the Vanguard of Research and Technology" organized on the occasion of the 170th anniversary of the National Technical University of Athens, Athens, Greece, December 2007.

Tsalikis, D.; Lempesis, N.; Boulougouris, G.C.; Theodorou, D.N. "On the Role of Inherent Structures in Glass-Forming Materials", Annual AIChE meeting, Philadelphia, PA, USA, November 2008.

Spyriouni, T.; Boulougouris, G.C.; Theodorou, D.N. "Sorption Equilibria of $CO_2$ in Atactic Polystyrene by Molecular Simulation", Annual AIChE meeting, Philadelphia, PA, USA, November 2008.

Romanos, N.; Theodorou, D.N. "Computer Simulations of Crystallization of Polymer Melts", 7th Panhellenic Scientific Conference in Chemical Engineering, Patras, Greece, June 2009.

Boulougouris, G.; Spyriouni, T.; Theodorou, D.N. "Development of a Computational Methodology for Predicting the Sorption of $CO_2$ in Atactic Polystyrene at High Pressures", 7th Panhellenic Scientific Conference in Chemical Engineering, Patras, Greece, June 2009.

Vyrkou, A.; Megariotis, G.; Pitouras, Z.; Lwygue, A.; Theodorou, D.N. "Atomistic and Mesoscopic Simulations of Liquid Crystalline Phases and Their Interfaces with Water", 7th Panhellenic Scientific Conference in Chemical Engineering, Patras, Greece, June 2009.

Megariotis, G.; Vyrkou, A.; Leygue, A.; Theodorou, D.N. "Systematic Development of a Coarse-Grained Model for 5CB (4-cyano-4'-pentyl biphenyl)", poster presentation, Faraday Discussion 144, *Multiscale Modeling of Soft Matter*, Groningen, The Netherlands, July 2009.

Vergadou, N.; Theodorou, D.N. "Microscopic Diffusion Mechanism of $CO_2$ in a Glassy Amorphous Polymer Matrix", poster presentation, Diffusion Fundamentals III conference, Athens, Greece, August 2009.

Pantatosaki, E.; Papadopoulos, G.K.; Theodorou, D.N. "Simulation Studies of $CH_4$, $CO_2$, $H_2$ and $D_2$ in FAU and MWW Framework Type Zeolites", poster presentation, Diffusion Fundamentals III conference, Athens, Greece, August 2009.

Sant, M.; Papadopoulos, G.K.; Theodorou, D.N. "Diffusion via the Space Discretization (DSD) Method to Study the Concentration Dependence of Self-Diffusion under Confinement", poster presentation, Diffusion Fundamentals III conference, Athens, Greece, August 2009.

Tsalikis, D.; Lempesis, N.; Boulougouris, G.C.; Theodorou, D.N. "Energy Lanscape-Based Study of Atomic Displacements in Glass Forming Materials", poster presentation, Diffusion Fundamentals III conference, Athens, Greece, August 2009.

Pantatosaki, E.; Papadopoulos, G.K.; Jobic, H.; Theodorou, D.N. "A Combined Atomistic Simulation and Quasielastic Neutron Scattering Study of the Low-Temperature Dynamics of Hydrogen and Deuterium Confined in NaX Zeolite", poster presentation, Diffusion Fundamentals III conference, Athens, Greece, August 2009.

Pazzona, F.G.; Sant, M.; Pantatosaki, E.; Papadopoulos, G.K.; Theodorou, D.N. "Analysis of Argon Diffusion in Zeolite Imidazolate Framework-8: Preliminary Calculations", poster presentation, Diffusion Fundamentals III conference, Athens, Greece, August 2009.

Anogiannakis, S.D.; Tzoumanekas, C.; Rousseau, B.; Theodorou, D.N. "Tube Segment Survival Probability from Computed Generated Trajectories: Onset of Tube Confinement", Annual European Rheology Conference, Göteborg, Sweden, April 2010.

Tzoumanekas, C.; Lahmar, F.; Rousseau, B.; Theodorou, D.N. "From Rods to Random Walks: Onset of Entanglements Revisited", poster presentation, Annual European Rheology Conference, Göteborg, Sweden, April 2010.

Megariotis, G.; Vyrkou, A.; Leygue, A. ; Theodorou, D.N. "Systematic Development of a Coarse-Grained Model for 5CB (4-cyano-4'-pentyl biphenyl)", poster presentation, 12th International Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD 2010), Suzhou, China, May 2010.

Romanos, N.A.; Theodorou, D.N. "Crystallization and Melting of Isotactic Polypropylene", poster presentation, 12th International Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD 2010), Suzhou, China, May 2010.

Pantatosaki, E.; Jobic, H.; Papadopoulos, G.K.; Theodorou, D.N. "Simulation and Experimental Study of $CH_4$ Sorption and Kinetics in FAU-type Zeolites and ZIF-8", poster presentation, 16th International Zeolite Conference and 7th International Mesostructured Materials Symposium (IZC16-IMMS7), Sorrento, Italy, July 2010.

Sant, M.; Papadopoulos, G.K.; Theodorou, D.N. "Study of the Self-Diffusivity of methane in ITQ-1 Zeolite via the Diffusion through Space Discretization (DSD) method", poster presentation, 16th International Zeolite Conference and 7th International Mesostructured Materials Symposium (IZC16-IMMS7), Sorrento, Italy, July 2010.

Romanos, N.; Theodorou, D.N. "Computer Simulations of Crystallization and Melting of the $\alpha 1$ Form of Oligomeric Isotactic Polypropylenes", 8th Panhellenic Scientific Conference in Chemical Engineering, Thessaloniki, Greece, May 2011.

Vogiatzis, G.G.; Voyiatzis, E.; Theodorou, D.N. "Mesoscopic Monte Carlo Simulations of Polymer-Matrix Nanocomposite Materials", 8th Panhellenic Scientific Conference in Chemical Engineering, Thessaloniki, Greece, May 2011.

Romanos, N.A.; Theodorou, D.N. "Molecular Simulations of the $\alpha 1$ Form of Isotactic Polypropylene for the Prediction of Melting Point $T_m$", Thermodynamics 2011 Conference, Athens, Greece, September 2011.

Ndoro, T.V.M.; Voyiatzis, E.; Böhm, M.C.; Theodorou, D.N.; Müller-Plathe, F. "Local Stress Distribution in a Polystyrene-Silica Nanocomposite System", Thermodynamics 2011 Conference, Athens, Greece, September 2011.

Vogiatzis, G.G.; Theodorou, D.N. “Chain Conformations in Polymer Nanocomposites: A Field Theory-Inspired Monte Carlo Simulation Approach”, NANO2012 XI International Conference on Nanostructured Materials, Rhodes, Greece, August 2012.

Vogiatzis, G.C.; Theodorou, D.N. “Local Polymer Dynamics in Polystyrene-$C_{60}$ Mixtures”, poster presentation, 9th Hellenic Polymer Society Conference, Thessaloniki, Greece, November 2012. **Presentation won one of the three best poster awards of the conference.**

Moorthi, K.; Kamio, K.; Ramos, J.; Theodorou, D.N. “Stucture and entanglements in short chain branched polyolefin melts”, 4th International Symposium on Slow Dynamics in Complex Systems, Tohoku University, Sendai, Japan, December 2012.

Mathioudakis, J.G.; Vogiatzis, G.G.; Theodorou, D.N. “Molecular Simulation of Nanocomposite Polymeric Materials at Multiple Time Scales”, poster presentation, 9th Panhellenic Scientific Conference in Chemical Engineering, Athens, Greece, May 2013.

Kolokathis, P.D.; Theodorou, D.N. “Reduction of the Dimensionality of the Local Free Energy Profiles of Benzene in the Zeolite Silicalite-1: Computation of Diffusion Coefficients Using Transition State Theory”, 9th Panhellenic Scientific Conference in Chemical Engineering, Athens, Greece, May 2013. **Presentation won the first prize for an oral presentation by a doctoral student in the conference.**

Skountzos, E.; Anastasiou, A.; Sabethai, S.; Mavrantzas, V.G.; Theodorou, D.N. “Polymer-graphene Nanocomposites: Atomistic Modeling and Simulation of Their Mechanical Properties”, 9th Panhellenic Scientific Conference in Chemical Engineering, Athens, Greece, May 2013.

Romanos, N.A.; Theodorou, D.N. “Study of the Rotator Phase of Isotactic Polypropylene and of its Crystalline Behavior Before Melting with the Molecular Dynamics Method”, poster presentation, 9th Panhellenic Scientific Conference in Chemical Engineering, Athens, Greece, May 2013.

Vogiatzis, G.G.; Megariotis, G.; Theodorou, D.N. “Multiscale Simulations of Polymer-Matrix Nanocomposites”, 10th International Conference on Nanosciences and Nanotechnologies, Thessaloniki, July 2013.

Ziogos, O.G.; Tsetseris, L.; Theodorou, D.N. Atomistic Simulations of Dipole Substituted peri-Hexabenzocoronene Molecular Crystals”, XXIX Panhellenic Conference of Solid State Physics and Materials Science, Athens, Greece, September 2013.

Mathioudakis, J.G.; Vogiatzis, G.G.; Theodorou, D.N. “Molecular Simulation of Nanocomposite Polymeric Materials at Multiple Time Scales”, poster presentation, XXIX Panhellenic Conference of Solid State Physics and Materials Science, Athens, Greece, September 2013.

Vogiatzis, G.G.; Megariotis, G.; Tzoumanekas, C.; Theodorou, D.N. “Polymer Network Simulations at a Mesoscopic Level”, FEMS EUROMAT 2013 European Congress and Exhibition on Advanced Materials and Processes, Seville, Spain, September 2013.

Megariotis, G.; Ziogos, O.G.; Theodorou, D.N. “Coarse-Graining of the Mesogen Hexa-n-dodecyl-hexa-peri-hexabenzocoronene (HBC-C12) and Hexabenzocoronene (HBC)”, 11th International Conference on Computational Methods in Science and Engineering (ICCMSE 2015), Athens, Greece, March 2015.

Kritikos, G.; Vogiatzis, G.G.; Theodorou, D.N. "Computational Study of the Dynamics of and Thermodynamics of Highly Confined Polyethylene", 10th Panhellenic Scientific Conference on Chemical Engineering, Patras, Greece, June 2015.

Mathioudakis, I.G.; Vogiatzis, G.G.; Tzoumanekas, C.; Theodorou, D.N. "Molecular modeling and simulation of polymer nanocomposites at multiple length scales", IEEE NANO 2015 Conference, Rome, Italy, July 2015.

Ziogos, O.G.; Theodorou, D.N. "Structural and Dynamical Properties of Nanographene Molecular Wires: a Molecular Dynamics Study", poster presentation, IEEE NANO 2015 Conference, Rome, Italy, July 2015.

Anogiannakis, S.; Theodorou, D.N.; Tzoumanekas, C. "Primitive Path Dynamics, Constraint Release and Contour Length Fluctuations in a Model Polyethylene Melt: A First Principles, Atomistic Simulation Study", 8th GRACM International Congress on Computational Mechanics, Volos, Greece, July 2015.

Megariotis, G.; Vogiatzis, G.G.; Theodorou, D.N. "Equation of State – Based Slip-Spring Model for Entangled Polymer Melt and Rubber Dynamics", 8th GRACM International Congress on Computational Mechanics, Volos, Greece, July 2015.

Kritikos, G.; Sgouros, A.; Vogiatzis, G.G.; Theodorou, D.N. "Molecular Dynamics Study of Polyethylene Under Extreme Confinement", International Conference on Mathematical Modeling in Physical Sciences 2016 (IC-MSQUARE 2016), Athens, Greece, May 2016.

Mathioudakis, I.; Vogiatzis, G.G.; Tzoumanekas, C.; Theodorou, D.N. "Molecular Modeling and Simulation of Atactic Polystyene/Amorphous Silica Nanocomposites", International Conference on Mathematical Modeling in Physical Sciences 2016 (IC-MSQUARE 2016), Athens, Greece, May 2016.

Megariotis, G.; Vogiatzis, G.G.; Schneider, L.; Müller, M.; Theodorou, D.N. "Mesoscopic Simulations of Crosslinked Polymer Networks", International Conference on Mathematical Modeling in Physical Sciences 2016 (IC-MSQUARE 2016), Athens, Greece, May 2016.

Ziogos, O.; Mathioudakis, I.; Theodorou, D.N. "Atomistic and Coarse-Grained Simulations of Hexabenzocoronene Crystals", International Conference on Mathematical Modeling in Physical Sciences 2016 (IC-MSQUARE 2016), Athens, Greece, May 2016.

Vogiatzis, G.; Theodorou, D.N. "Multiscale Simulations of Polymer-Matrix Nanocomposites", European Congress on Computational Methods in Applied Sciences and Engineering, Crete, Greece, June 2016 (G. Vogiatzis's Ph.D. thesis was selected as the best 2015 thesis from NTUA for participation in the 2016 Ph.D. ECCOMAS Olympiad).

Tzounis, P.G.; Anogiannakis, S.; Theodorou, D.N. "Atomistic Simulations of Oligomers Used in Directed Self-Assembly Lithography: Estimation of the Interaction Parameter $\chi$", poster presentation, International Symposium on Directed Self-Assembly, Grenoble, France, October 2016.

Tzounis, P.G.; Anogiannakis, S.; Theodorou, D.N. "Single Unperturbed Chain Monte Carlo Algorithm: A General Methodology for Estimating the Dimensions of Unperturbed Polymer

Chains", poster presentation, International Symposium on Directed Self-Assembly, Grenoble, France, October 2016.

Sgouros, A.; Lakkas, A.; Megariotis, G.; Vogiatzis, G.; Theodorou, D.N. "Multiscale Modeling of Interfacial Polymer Systems", 11th Hellenic Polymer Society International Conference, Ioannina, Greece, November 2016.

Tzounis, P.-N.; Anogiannakis, S.D.; Koulierakis, E. Theodorou, D.N. "Atomistic Simulations of Oligomers Used in Directed Self-Assembly Lithography", 11th Panhellenic Scientific Conference on Chemical Engineering, Thessaloniki, Greece, May 2017.

Tzounis, P.-N.; Anogiannakis, S.D.; Theodorou, D.N. "General Methodology for Estimating the Dimensions of Polymer Chains Based on Atomistic Monte Carlo Simulations of Single Unperturbed Chains", poster presentation, poster presentation, 11th Panhellenic Scientific Conference on Chemical Engineering, Thessaloniki, Greece, May 2017.

Ziogos, O.-G.; Theodorou, D.N. "Simulations of Nanographene Molecular Crystals", 11th Panhellenic Scientific Conference on Chemical Engineering, Thessaloniki, Greece, May 2017.

Constantinopoulos, S.; Ziogos, O.-G.; Theodorou, D.N. "Atomistic Simulations of Discotic Liquid Crystals of Nanographene", poster presentation, 11th Panhellenic Scientific Conference on Chemical Engineering, Thessaloniki, Greece, May 2017.

Bardas, Ch. G.; Ziogos, O.-G.; Theodorou, D.N. "Atomistic Simulations of Nanocomposite Materials Consisting of Carbon Nanotubes in Polymer Matrices", poster presentation, 11th Panhellenic Scientific Conference on Chemical Engineering, Thessaloniki, Greece, May 2017.

Perdikari, T.M.; Ziogos, O.-G.; Theodorou, D.N. "Atomistic Simulations of Lamellar Nanostructures of Amphiphilic Discotic Molecules", poster presentation, 11th Panhellenic Scientific Conference on Chemical Engineering, Thessaloniki, Greece, May 2017.

Lakkas, A.; Sgouros, A.; Kissas, G.; Liveris, D.; Megariotis, G.; Theodorou, D. "Self-Consistent Field Theory in the Study of Polymer Interfaces", 11th Panhellenic Scientific Conference on Chemical Engineering, Thessaloniki, Greece, May 2017.

Megariotis, G.; Abdolhadi, V.; Mavromoustakos, T.; Theodorou, D. "Molecular Simulations of Anti-Hypertension Drugs in Lipid Membranes", poster presentation, 11th Panhellenic Scientific Conference on Chemical Engineering, Thessaloniki, Greece, May 2017.

Megariotis, G.; Vogiatzis, G.; Sgouros, A.; Lakkas, A.; Theodorou, D. "Presentation of a Computational Code for Mesoscopic Simulations of Polymer Networks", poster presentation, 11th Panhellenic Scientific Conference on Chemical Engineering, Thessaloniki, Greece, May 2017.

Kallivokas, S.V.; Sgouros, A.P.; Theodorou, D.N. "Study of Structural and Thermodynamic Properties of Epoxy Resins for Reinforcement of Mechanical Properties", poster presentation, 11th Panhellenic Scientific Conference on Chemical Engineering, Thessaloniki, Greece, May 2017.

Romanos, N.; Theodorou, D.N. "Study of the Crystalline Behavior of the α2 Crystal Form of Oligomeric Isotactic Polypropylene Prior to Melting With the Molecular Dynamics (MD) Method", poster presentation, 11th Panhellenic Scientific Conference on Chemical Engineering, Thessaloniki, Greece, May 2017.

Megariotis, G.; Mavromoustakos, T.; Theodorou, D.N. "A Molecular Dynamics Study of Irbesartan in a Lipid Membrane", Scienomics Scimeeting and Group of Scientific Excellence meeting, NCSR "Demokritos", Athens, Greece, June 2017.

Sgouros, A.; Megariotis, G.; Lakkas, A.; Theodorou, D.N. "Multiscale Modeling of Polymer Systems with Interfaces", 15th Euromat Conference, Thessaloniki, Greece, September 2017.

Lakkas, A.; Sgouros, A.; Megariotis, Theodorou, D.N. "Self-Consistent Field Model of Inhomogeneous Polymer Systems: Solution by the Finite Element Method", 15th Euromat Conference, Thessaloniki, Greece, September 2017.

Megariotis, G.; Sgouros, A.; Lakkas, A.; Theodorou, D.N. "Mesoscopic Simulations of Elastomeric Materials", 15th International Conference on Nanosciences and Nanotechnologies (NN15), Thessaloniki, Greece, July 2018.

Revelas, C.J.; Sgouros, A.P.; Theodorou, D.N. "Multiscale Modeling of Polymer-Nanoparticle Systems", CECAM Mixed-Gen series on Multiscale Simulation of Complex Materials (virtual workshop), chosen for oral presentation by the organizers, October 2021.

Vogiatzis, G.; van Breemen, L.C.A.; Hütter, M.; Theodorou, D.N. "Molecular Simulations of Multi-Process Aging of Polymer Glasses: Current Status and Perspectives", 13th Hellenic Polymer Society International Conference (virtual event), December 2021.

Kallivokas, S.; Sgouros, A.P.; Theodorou, D.N. "Towards a New Equation for the Interfacial Failure of Nanocomposites", 13th Panhellenic Scientific Conference on Chemical Engineering, Patras, Greece, June 2022 (**won best oral presentation award in the area of Polymers and Nanocomposites**)

Mikaelian, G.; Pitterou, I.; Detsi, A.; Megariotis, G.; Theodorou, D.N. "Molecular Simulations of Dopamine – β-Cyclodextrin Complexes in Aqueous Environments", 13th Panhellenic Scientific Conference on Chemical Engineering, Patras, Greece, June 2022.

Loukas, A.T.; Mikaelian, G.; Megariotis, G.; Theodorou, D.N. "Molecular Simulations of Diphenhydramine in Hydrated Lipid Bilayers", poster presentation, 13th Panhellenic Scientific Conference on Chemical Engineering, Patras, Greece, June 2022.