DOROS NICOLAS THEODOROU
Professor
Department of Materials Science and Engineering
School of Chemical Engineering
National Technical University of Athens
9 Heroon Polytechniou Street, Zografou Campus
GR-157 80 Athens, Greece
Tel. +30 210 772 3157, Fax +30 210 772 3112
E-mail *doros@central.ntua.gr*
http://comse.chemeng.ntua.gr

Research Interests Computer modeling of matter. Application of statistical mechanics, thermodynamics, and transport phenomena for the elucidation of structure-processing-property relations in materials. Multiscale modeling and simulation strategies. Polymer science and engineering. Polymer-matrix nanocomposites. Interfacial phenomena. Self-assembly in soft matter systems. Zeolites and other nanoporous solids.

Personal Data Born 29 October, 1957 in Athens, Greece.
Married, one child

Education Diploma, National Technical University of Athens, Greece, 1982, Chem. Engineering.
Master of Science, Massachusetts Institute of Technology, 1983, Chem. Engineering.
Ph.D., Massachusetts Institute of Technology, 1985, Chemical Engineering.

Employment

	Massachusetts Institute of Technology	Cambridge, MA, USA
1981-1985	Research Assistant, Chemical Engineering Department.	
Spring 1985	Teaching Assistant, graduate thermodynamics, Chemical Engineering Department.	
	Hellenic Naval Academy	Piraeus, Greece
1985-1986	Instructor in computer programming and computer center administrator (mil. service).	
	University of California, Berkeley	Berkeley, CA, USA
1986-1990	Assistant Professor of Chemical Engineering.	
1990-1994	Associate Professor of Chemical Engineering.	
1994-1995	Professor of Chemical Engineering.	
	Lawrence Berkeley Laboratory	Berkeley, CA, USA
1986-1995	Associated Faculty, Polymers Program, Center for Advanced Materials, Division of Materials Sciences. Project Leader, Polymer/Substrate Interactions.	
	University of Patras	Patras, Greece
1991-1994	Associate Professor of Chemical Engineering.	
1994-2002	Professor of Chemical Engineering.	
	National Technical University of Athens	Athens, Greece
2002-	Professor of Chemical Engineering.	
	Institute of Chemical Engineering and High Temperature Chemical Processes (ICE/HT-FORTH)	Patras, Greece
1991-2007	Adjunct Senior Researcher.	
	National Center for Scientific Research "Demokritos"	Athens, Greece
Spring 1992	Visiting Professor, Physical Chemistry Institute.	
1993-	Collaborating Researcher	

1993-2005 Director, Molecular Modeling of Materials Laboratory.

Classes Taught at U.C. Berkeley

undergraduate Chemical Engineering Thermodynamics (with J.M. Prausnitz), Transport Processes (Heat and Mass), Polymer Science and Engineering, Chemical Engineering Laboratory.

graduate Thermodynamics for Chemical Product and Process Design (with J.M. Prausnitz).
Applied Molecular Theory for Chemical Engineers (with Arup K. Chakraborty).

Classes Taught at the University of Patras

undergraduate Mass and Energy Balances, Physical Chemistry II, Chemical Thermodynamics I and II, Advanced Thermodynamics.

graduate Chemical Engineering Thermodynamics, Statistical Mechanics and Molecular Simulation, Physical Chemistry of Polymers, Statistical Mechanics of Polymers (with A. Dondos, D. Photinos, M. Kosmas, A. Terzis)

Classes Taught at the National Technical University of Athens

undergraduate Physical Chemistry II (Structure and States of Matter), Structure-Property Relations in Materials, Polymer Science, Connecting Microscopic and Macroscopic Properties via Computation

graduate Molecular Simulations of Materials

Classes Taught at NCSR "Demokritos"

graduate Topics in Statistical Mechanics and Thermodynamics of Molecular Systems and Applications to the Molecular Simulation of Materials Using Supercomputers.
Molecular Simulations of Physicochemical Systems (with A.Z. Panagiotopoulos).
Polymer Physics and Physical Chemistry (with I. Economou, C. Tsenoglou, N. Hadjichristidis, and J. Petropoulos)

Honors

Salutatorian, Summa cum Laude, Ancient Greek Prize, Dolashik Prize, Athens College, 1976.
Entrance examination award, National Technical University of Athens, 1976.
Condoulis and Thomaides awards, National Technical University of Athens, 1978-1981.
17 November 1973 prize, Technical Chamber of Greece, 1977-1981.
Chrysovergis prize, National Technical University of Athens, 1982.
Gilliland Fellowship, Massachusetts Institute of Technology, U.S.A., 1981-1982.
Scholarship of the Bodossakis Foundation, 1981-1984.
Shell Faculty Career Initiation Grant, U.S.A., 1986-1988.
Du Pont Young Faculty Grant, U.S.A., 1989-1991.
Presidential Young Investigator Award, U.S. National Science Foundation, 1988-1992.
Allan P. Colburn Memorial Lectureship, Department of Chemical Engineering, University of Delaware, Newark, Delaware, U.S.A., October 1992.
Ernest W. Thiele Lectureship, Department of Chemical Engineering, University of Notre Dame, Notre Dame, Indiana, U.S.A., September 1993.
Robert W. Vaughan Lecture, Department of Chemical Engineering, California Institute of Technology, Pasadena, California, U.S.A., March 1994.
Science Award of the Bodossakis Foundation in Chemistry, 1996.
Invitation to the international conference *Scientia Europaea*, organized by the Institut de France and the Fondation Rhône-Poulenc, September 1998.
Danckwerts Lecture, awarded by the AIChE, IChemE, EFCE, and the Editors of *Chemical Engineering*

Science, AIChE Annual Meeting, San Francisco, California, U.S.A., November 2006.
Dick Medema Award in Polymer Science and Technology, awarded by the Dutch PTN (Polymer Technology in the Netherlands), Lunteren, The Netherlands, February 2009.
Bird-Stewart-Lightfoot Lectureship, Department of Chemical and Biological Engineering, University of Wisconsin-Madison, May 2013.
Elected to the National Academy of Engineering of the U.S.A., February 2015.
John M. Prausnitz Award in Applied Chemical Thermodynamics, Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD 2016), Porto, Portugal, May 2016.
John M. Prausnitz AIChE Institute Lecture, AIChE Annual Meeting, San Francisco, California, USA, November 2016.
European Materials Medal, awarded by the Federation of European Materials Research Societies (FEMS), Euromat 2017 conference, Thessaloniki, Greece, September 2017.
DSM Life Time Achievement Award in Materials Sciences, DYFP2018 Conference, Kerkrade, The Netherlands, March 2018.
"Alkiviades Ch. Payatakes" Distinguished Lecture, FORTH/ICE-HT, Patras, Greece, December 2018.
2018 Guggenheim Medal of the Institution of Chemical Engineers, UK for significant contribution to Thermodynamics and/or Complex Fluids, Thermodynamics 2019 conference, Punta Umbría, Spain, June 2019.
2022 FOMMS Medal for "profound and lasting contributions to the development of computational methods and their application to the field of molecular-based modeling and simulation"
Included in *Who's Who in the World*, *Who's Who in Science and Engineering*, *Men and Women of Science*, *Men of Achievement*, *European Biographical Directory*.

Professional Activities

Member of the National Council of Research, Technology, and Innovation of Greece (ESETEK), 2020-

Member, Scientific Steering Committee, PRACE (Partnership for Advanced Computing in Europe), 2020-

Member, Products and Processes Engineering Panel (PE8) 2015, 2017, 2019 and Materials Engineering Panel (PE11) 2021, Advanced Grant Evaluation, European Research Council.

Member (2011-) and Vice President (2021-) of the Board, Bodossakis Foundation.

Member of the Scientific Council for the National Competition "Greece is Innovating!", organized by the Association of Greek Industries (SEB) and Eurobank, 2012-2013.

Member of the National Council of Research and Technology of Greece (ESET), 2010-2013.

Member of the Management Board, Institute of Accelerating Systems and Applications (IASA), Athens, Greece, 2009-

Member of the Sectorial Scientific Council for Physics, Chemistry, and Materials, National Council of Research and Technology of Greece,2003-2004.

National Representative of Greece to the HRM (Human Resources and Mobility) Program Committee, Directorate General XII of the European Commission, 2003-2004.

National Representative of Greece to the IHP (Improving Human Potential) Program Committee, Directorate General XII of the European Commission, 2000-2002.
National Representative of Greece to the TMR (Training and Mobility of Researchers) Program Committee, Directorate General XII of the European Commission, 1995-1998.

Visiting Researcher, Institute of Theoretical Physics, University of California, Santa Barbara, U.S.A. (Program on Quantitative Methods in Materials Research), April-May 1997.

International Advisory Board, *Molecular Systems Design and Engineering*, 2017-
Editorial Board, *Journal of Multiscale Modelling*, 2009-
Editorial Committee Member, *Annual Review in Chemical and Biomolecular Engineering*, 2008-2015
Editorial Board, *Molecular Physics*, 2006-2012
Editorial Advisory Board, *Macromolecules*, 2005-2007
Editorial Board, *Microporous and Mesoporous Materials*, 2004-2022
Editorial Board, *Soft Materials*, 2002-2009
International Advisory Board, *Chemical Engineering Science*, 2000-2018
Editorial Board, *Computational and Theoretical Polymer Science*, 1996-2002
Editorial Board, *Molecular Simulation*, 1994-2001
Editorial Board, *Journal of Computer-Aided Materials Design*, 1993-2007
Editorial Board, *Die Makromolekulare Chemie: Theory and Simulation*, 1992-1995

Guest editor, with Mark J. Biggs, 2013 Danckwerts Special Issue on Molecular Modeling in Chemical Engineering, *Chemical Engineering Science*, 2015.

Co-editor, *Diffusion in Micropores*, special issue of the journal *Microporous and Mesoporous Materials*, honouring Prof. Dr. Jörg Kärger of the University of Leipzig, 2009.

Editor, Symposium in Print on Molecular Modeling, published by *Chemical Engineering Science*, 1994.

Member of the International Advisory Committee, 9th Liquid Matter Conference, Ljubljana, Slovenia, July 2017.

Member of the International Advisory Board, Conference on Properties and Phase Equilibria for Product and Process Design, 14th edition (PPEPPD 2016), Porto, Portugal, May 22-26, 2016 and 13th edition (PPEPPD 2013), May 26-30, Iguazu Falls, Argentina, May 26-30, 2013.

Member of the selection committee, Ilya Prigogine Prize in Thermodynamics 2021, 2019, 2017, 2015.

Member of the Scientific Committee, Joint European Thermodynamics Conference, 13th edition (JETC 2015), Nancy, France, May 20-22, 2015 and 12th edition (JETC 2013), Brescia, Italy, July 1-5, 2013.

Member of the International Organizing Committee, Conference on Properties and Phase Equilibria for Product and Process Design, 12th edition (PPEPPD 2010), Suzhou, China, and 10th edition (PPEPPD 2004), Snowbird, Utah, May 2004.

Scientific Advisor, School and Conference on Multiscale Modeling and Simulations of Hard and Soft Materials, Bangalore, India, December 2009.

Co-chairman, Diffusion Fundamentals III conference, Athens, Greece, August 23-26, 2009.

Co-organizer, Faraday Discussion 144, "Multiscale Modeling of Soft Matter", Groningen, The Netherlands, July 20-22, 2009.

Chairman of the International Organizing Committee, 11th edition of the Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD 2007), Hersonissos, Crete, Greece, May 20-25, 2007.

Session Organizer, "Coarse-Grained Models for Polymers", SIMU Conference "Bridging the Scales", Genova, Italy, August 2004.

Co-organizer, 19th European Seminar on Applied Thermodynamics, Santorini, Greece, September 2002.

Co-organizer, SIMU-CECAM Workshop on Multiscale Modeling of Materials: Methods, Algorithms, and Unsolved Problems, Heraklion, Crete, Greece, July 2001.

Co-organizer, CECAM-ESF Workshop on Computer Simulations of Polymer Blends and Copolymer Systems, Lyon, France, September 13-15, 1999.

Co-chairman, ACS Workshop on Molecular Modeling of Polymers, Isle of Palms, SC, USA, March 1998.

Chairman of the Scientific Committee, 6th European Polymer Federation Symposium on Polymeric Materials, Aghia Pelaghia, Crete, Greece, October 1996.

Co-organizer, Symposium on Modeling and Computer Simulation of Polymers, Division of Polymer Chemistry, National Meeting of the American Chemical Society, San Francisco, California, April 1992.

Co-organizer, Symposium on Structure and Mobility in Polymer Solids, 2nd Topical Conference on Emerging Technologies in Materials, 1989 Annual Meeting of the American Institute of Chemical Engineers, San Francisco, California, November 1989.

Scientific Advisor, Molecular Simulations Inc./Accelrys, San Diego, CA, USA and Cambridge, UK, 1999-2005. Member of Scientific advisory board, Scienomics SARL, Paris, France, 2005-. Consultant, DSM Research, Geleen, The Netherlands, 2001-. Consultant, E.I. du Pont de Nemours & Co., W.R. Grace & Co.-Conn., BFGoodrich Co., Biosym Technologies, Inc., Oxford Molecular Ltd., 1989-1995.

Member, Committee for Strategic Planning, School of Chemical Engineering, National Technical University of Athens, 2019-.

Member of the Senate Committee on Postgraduate Education of the National Technical University of Athens, 2015-2019.

Member of the Undergraduate Curriculum Committee of the School of Chemical Engineering at the National Technical University of Athens, 2015-2016.

Member of the Senate Committee on Basic Research of the National Technical University of Athens, 2006-.

Chairman of the Steering Committee (2018-) and instructor (2012-), Interpartmental Program of Graduate Studies “Computational Mechanics”, NTU Athens.

Instructor, Interpartmental Program of Graduate Studies “Materials Science and Technology”, NTU Athens, 2014–

Member of Steering Committee and Instructor, Interpartmental Program of Graduate Studies “Microsystems and Nanodevices”, NTU Athens, 2006-.

Member of Steering Committee and Instructor, Interpartmental Program of Graduate Studies “Mathematical Modeling in Modern Technologies and in Financial Engineering”, NTU Athens, 2003-.

Member of the Steering Committee of the European Network ‘‘Challenges in Molecular Simulation: Bridging the Length- and Time-Scale Gap’’ (SIMU), supported by the ESF, 1999-2004.

Member of the steering committee for the establishment of a supercomputer centre in Greece, National Hellenic Research Foundation, 1999-2000.

Member of the provisional general assembly of the newly formed Materials Science Department at the University of Patras, 1999-2002.

Instructor in the Interdepartmental Program of Graduate Studies ‘‘Polymer Science and Engineering’’, University of Patras, 1998-2002.

Instructor in the program of graduate studies ‘‘Polymer Science and Its Applications’’, University of Athens, 1998-2002.

Instructor in the Third Summer School in Chemistry (SSC-3) ‘‘Topics in Polymer Chemistry’’, Socrates Program, University of Patras, July 2000.

Reviewer of instructional material prepared for the Hellenic Open University, 1998-2000

Member of Ph.D. examination committees at Imperial College London (UK), at the Universities of Groningen (NL), Eindhoven (NL), Twente (NL), Delft (NL), Leipzig (DE), Dortmund (DE), Oslo (NO), Cagliari and Sassari (IT), at the Indian Institute of Science, Bangalore, at the Indian Institute of Technology, Bombay, at the Royal Melbourne Institute of Technology (RMIT), Australia, at the University of Wollongong and at Deakin University, Australia, at the National University of Singapore (SG), at the Universities of Patras, Athens, Thessaloniki, Crete, Ioannina, and at NTU Athens. Member of jury for awarding a Habilitation á Diriger des Recherches at the Université de Savoie, France.

Reviewer of research proposals submitted to the following origanizations: National Science Foundation (USA), INTAS Program, DGXII of the European Union, Netherlands Foundation for Chemical Research (SON), Dutch *Softlink* Program, A.C.S. Petroleum Research Fund (U.S.A.), CECAM (Centre Européen de Calcul Atomique et Moléculaire), PRACE (Partnership for Advanced Computing in Europe), General Secretariat of Research and Technology of Greece, Research Commission of the ETH-Zürich, Research Committees of the Universities of Ioannina and Crete and of the National Technical University of Athens.

Referee of research articles submitted for publication to the journals *Proceedings of the National*

Academy of Sciences USA , Macromolecules, Journal of Chemical Physics, Journal of Physical Chemistry B, Langmuir, Accounts of Chemical Research, Physical Chemistry Chemical Physics, Chemical Communications, Molecular Physics, Microporous and Mesoporous Materials, Journal of Rheology, A.I.Ch.E. Journal, Chemical Engineering Science, J. Polymer Sci. B: Polymer Physics, Macromolecular Theory and Simulations, Theoretical and Computational Polymer Science, Polymers, Composites, Technika Chronika.

Member, American Institute of Chemical Engineers, American Chemical Society, Technical Chamber of Greece, Athens College Alumni Association.

Languages Greek, English, German, French.

Personal Interests Music (playing the piano), literature, traveling, swimming.

PUBLICATIONS

A. Research Papers

1. Theodorou, D.N.; Wei, J. "Diffusion and Reaction in Blocked and High Occupancy Zeolite Catalysts" *J.Catal*. **1983**, *83*, 205-224.

2. Theodorou, D.N.; Suter, U.W. "Geometrical Considerations in Model Systems With Periodic Boundaries" *J.Chem.Phys*. **1985**, *82*, 955-966.

3. Theodorou, D.N.; Suter, U.W. "Shape of Unperturbed Linear Polymers; Polypropylene" *Macromolecules* **1985**, *18*, 1206-1214.

4. Theodorou, D.N.; Suter, U.W. "Detailed Molecular Structure of a Vinyl Polymer Glass" *Macromolecules* **1985**, *18*, 1467-1478.

5. Theodorou, D.N.; Suter, U.W. "Atomistic Modeling of Mechanical Properties of Polymeric Glasses" *Macromolecules* **1986**, *19*, 139-154.

6. Theodorou, D.N.; Suter, U.W. "Local Structure and the Mechanism of Response to Elastic Deformation in a Glassy Polymer" *Macromolecules* **1986**, *19*, 379-387.

7. Theodorou, D.N. "Lattice Models for Bulk Polymers at Interfaces", *Macromolecules* **1988**, *21*, 1391-1400.

8. Theodorou, D.N. "Structure and Thermodynamics of Bulk Homopolymer/Solid Interfaces: A Site Lattice Model Approach" *Macromolecules* **1988**, *21*, 1400-1410.

9. Theodorou, D.N. "Structure and Thermodynamic Properties of Bulk Copolymers and Surface Active Polymers at Interfaces 1.Theory" *Macromolecules* **1988**, *21*, 1411-1421.

10. Theodorou, D.N. "Structure and Thermodynamic Properties of Bulk Copolymers and Surface Active Polymers at Interfaces 2.Results for Some Representative Chain Architectures" *Macromolecules* **1988**, *21*, 1422-1436.

11. Mansfield, K.F.; Theodorou, D.N. "Interfacial Structure and Dynamics of Macromolecular Liquids: A Monte Carlo Simulation Approach" *Macromolecules* **1989**, *22*, 3143-3152.

12. Theodorou, D.N. "Variable Density Model of Polymer Melt Surfaces: Structure and Surface Tension" *Macromolecules* **1989**, *22*, 4578-4589.

13. Theodorou, D.N. "Variable Density Model of Polymer Melt/Solid Interfaces: Structure, Adhesion Tension, and Surface Forces" *Macromolecules* **1989**, *22*, 4589-4597.

14. June, R.L.; Bell, A.T.; Theodorou, D.N. "Prediction of Low Occupancy Sorption of Alkanes in Silicalite" *J.Phys.Chem.* **1990**, *94*, 1508-1516.

15. Mansfield, K.F.; Theodorou, D.N. "Atomistic Simulation of a Glassy Polymer Surface" *Macromolecules* **1990**, *23*, 4430-4445.

16. June, R.L.; Bell, A.T.; Theodorou, D.N. “Molecular Dynamics Study of Methane and Xenon in Silicalite” *J. Phys. Chem.* **1990**, *94*, 8232-8240; erratum *J. Phys. Chem.* **1991**, *95*, 1014.

17. Dodd, L.R.; Theodorou, D.N. “Analytical Treatment of the Volume and Surface Area of Molecules Formed by an Arbitrary Collection of Unequal Spheres Intersected by Planes” *Molec.Phys.* **1991**, *72*, 1313-1345.

18. Mansfield, K.F.; Theodorou, D.N. "Atomistic Simulation of a Glassy Polymer/Graphite Interface” *Macromolecules* **1991**, *24*, 4295-4309.

19. Snurr, R.Q.; June, R.L.; Bell, A.T.; Theodorou, D.N. “Molecular Simulations of Methane Adsorption in Silicalite" *Molecular Simulation* **1991**, *8*, 73-92.

20. June, R.L.; Bell, A.T.; Theodorou, D.N. “Transition State Studies of Xenon and SF_6 Diffusion in Silicalite” *J. Phys. Chem.* **1991**, *95*, 8866-8878.

21. Mansfield, K.F.; Theodorou, D.N. “Molecular Dynamics Simulation of a Glassy Polymer Surface” *Macromolecules* **1991**, *24*, 6283-6294.

22. Lonsinger, S.R.; Chakraborty, A.K.; Theodorou, D.N.; Bell, A.T. “The Effects of Local Structural Relaxation on Aluminum Siting Within H-ZSM-5” *Catal. Lett.* **1991**, *11*, 209-217.

23. June, R.L.; Bell, A.T.; Theodorou, D.N. “Molecular Dynamics Studies of Butane and Hexane in Silicalite” *J. Phys. Chem.*, **1992**, *96*, 1051-1060.

24. Dodd, L.R.; Boone, T.D.; Theodorou, D.N. “A Concerted Rotation Algorithm for Atomistic Monte Carlo Simulation of Polymer Melts and Glasses” *Molec.Phys.* **1993**, *78*, 961-996.

25. Theodorou, D.N.; Dodd, L.R.; Boone, T.D.; Mansfield, K.F. “Stress Tensor in Model Polymer Systems With Periodic Boundaries” *Makromol.Chem., Theory Simul.* **1993**, *2*, 191-238.

26. Sevick, E.M.; Bell, A.T.; Theodorou, D.N. “A Chain of States Method for Investigating Infrequent Event Processes Occurring in Multistate, Multidimensional Systems” *J. Chem. Phys.*, **1993,** *98*, 3196-3212.

27. Maginn, E.J.; Bell, A.T.; Theodorou, D.N. “Transport Diffusivity of Methane in Silicalite from Equilibrium and Nonequilibrium Simulations” *J. Phys. Chem.* **1993**, *97*, 4173-4181.

28. Cook, S.J.; Chakraborty, A. K.; Theodorou, D.N., Bell, A.T. “Structural and Electronic Features of the Brönsted Acid Site in H-ZSM-5” *J. Phys. Chem.* **1993**, *97*, 6679-6685.

29. Greenfield, M.L.; Theodorou, D.N. “Geometric Analysis of Diffusion Pathways in Glassy and Melt Atactic Polypropylene” *Macromolecules* **1993**, *26*, 5461-5672.

30. Snurr, R.Q.; Bell, A.T.; Theodorou, D.N. “Prediction of Adsorption of Aromatic Hydrocarbons in Silicalite from Grand Canonical Monte Carlo Simulations With Biased Insertions”, *J. Phys. Chem.* **1993**, *97*, 13742-13752.

31. Rapold, R.F.; Suter, U.W.; Theodorou, D.N. "Static Atomistic Modeling of the Structure and Ring Dynamics of Bulk Amorphous Polystyrene" *Macromol. Theory Simul.* **1994**, *3*, 19-43.

32. Snurr, R.Q.; Bell, A.T.; Theodorou, D.N. "A Hierarchical Atomistic/Lattice Simulation Approach for the Prediction of Adsorption Thermodynamics of Benzene in Silicalite" *J. Phys. Chem.* **1994**, *98*, 5111-5119.

33. Snurr, R.Q.; Bell, A.T.; Theodorou, D.N. "Investigation of the Dynamics of Benzene in Silicalite Using Transition-State Theory" *J.Phys.Chem.* **1994**, *98*, 11948-11961.

34. Maginn, E.J.; Bell, A.T.; Theodorou, D.N. "Sorption Thermodynamics, Siting and Conformation of Long *n*-Alkanes in Silicalite as Predicted by Configurational-Bias Monte Carlo Integration" *J.Phys.Chem.* **1995**, *99*, 2057-2079.

35. Kyrlidis, A.; Cook, S.J.; Chakraborty, A.C.; Bell, A.T.; Theodorou, D.N. "Electronic Structure Calculations of Ammonia Adsorption in H-ZSM-5 Zeolites" *J.Phys.Chem.* **1995**, *99*, 1505-1515.

36. Fischel, L.B.; Theodorou, D.N. "Self-Consistent Field Model of the Polymer/Diblock Copolymer/Polymer Interface" *J. Chem. Soc., Faraday Trans.* **1995**, *91*, 2381-2402.

37. Pant, P.V.K.; Theodorou, D.N. "Variable Connectivity Method for the Atomistic Monte Carlo Simulation of Polydisperse Polymer Melts" *Macromolecules* **1995**, *28*, 7224-7234.

38. Chassapis, C.S.; Petrou, J.K.; Petropoulos, J.H.; Theodorou, D.N. "Analysis of Computed Trajectories of Penetrant Micromolecules in a Simulated Polymeric Material" *Macromolecules* **1996**, *29*, 3615-3624.

39. Maginn, E.J.; Bell, A.T.; Theodorou, D.N. "Dynamics of Long n-Alkanes in Silicalite: A Hierarchical Simulation Approach" *J.Phys.Chem.* **1996**, *100*, 7155-7173.

40. 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" *Macromolecules* **1997**, *30*, 4744-4755.

41. Greenfield, M.L.; Theodorou, D.N. "Coupling of Penetrant and Polymer Motions During Small- Molecule Diffusion in a Glassy Polymer" *Molecular Simulation* **1997**, *19*, 329-361.

42. Provata, A.; Prassas, V.D.; Theodorou, D.N. "Surface Tension and Phase Coexistence Properties of the Lattice Fluid from a Virtual Site Removal Monte Carlo Strategy" *J. Chem. Phys.* **1997**, *107*, 5125-5140.

43. Fischel, L. B.; Newman, J.; Theodorou, D. N. ''Segment Density of a Block Copolymer Chain Tethered at Both Ends'' *J. Chem. Soc. Faraday Trans.* **1997**, *93*, 4355-4370.

44. Gray-Weale, A. A.; Henchman, R. H.; Gilbert, R. G.; Greenfield, M. L.; Theodorou, D. N.''Transition-State Theory Model for the Diffusion Coefficients of Small Penetrants in Glassy Polymers'' *Macromolecules* **1997**, *30*, 7296-7306.

45. Spyriouni, T.; Economou, I. G.; Theodorou, D. N. ‘‘Molecular Simulation of the Pure *n*-Hexadecane Vapor-Liquid Equilibria at Elevated Temperature’’ *Macromolecules* **1998**, *31*, 1430-1431.

46. Boulougouris, G.C.; Economou, I.G.; Theodorou, D.N. ‘‘Engineering a Molecular Model for Water Phase Equilibrium over a Wide Temperature Range’’ *J. Phys. Chem. B* **1998**, *102*, 1029-1035.

47. Mavrantzas, V.G.; Theodorou, D.N. ‘‘Atomistic Simulation of Polymer Melt Elasticity: Calculation of the Free Energy of an Oriented Polymer Melt’’ *Macromolecules* **1998**, *31*, 6310-6332.

48. Janssen, R.H.C.; Bomont, J.-M.; Theodorou, D.N., Raptis, S.; Papadopoulos, M.G. ‘‘Computer Simulation of the Linear and Nonlinear Optical Properties of Liquid Benzene: Its Local Fields, Refractive Index and 2nd Nonlinear Susceptibility’’ *J. Chem. Phys.* **1999**, *110*, 6463-6474.

49. Ullner, M. , Staikos, G.; Theodorou, D.N. ‘‘Monte Carlo Simulations of a Single Polyelectrolyte in Solution: Activity Coefficients of the Simple Ions and Application to Viscosity Measurements’’ *Macromolecules* **1998**, *31*, 7921-7933.

50. Spyriouni, T.; Economou, I.G.; Theodorou, D.N. ‘‘Phase Equilibria of Mixtures Containing Chain Molecules Through a Novel Simulation Scheme’’ *Phys. Rev. Lett.* **1998**, *80*, 4466-4469.

51. Harmandaris, V.A.; Mavrantzas, V.G.; Theodorou, D.N. ‘‘Atomistic Molecular Dynamics Simulation of Polydisperse Linear Polyethylene Melts’’ *Macromolecules* **1998**, *31*, 7934-7943.

52. Antoniadis, S.J.; Samara, C.T.; Theodorou, D.N. ‘‘Molecular Dynamics of Atactic Polypropylene Melts’’ *Macromolecules* **1998**, *31*, 7944-7952.

53. Greenfield, M.L.; Theodorou, D.N. ‘‘Molecular Modeling of Methane Diffusion in Glassy Atactic Polypropylene via Multidimensional Transition State Theory’’ *Macromolecules* **1998**, *31*, 7068-7090.

54. Errington, J.R.; Boulougouris, G.C.; Economou, I.G.; Panagiotopoulos, A.Z.; Theodorou, D.N. ‘‘Molecular Simulation of Phase Equilibria for Water-Methane and Water-Ethane Mixtures’’ *J. Phys. Chem. B* **1998**, *102*, 8865-8873.

55. Kopsias, N.P.; Theodorou, D.N. ‘‘Elementary structural transitions in the amorphous Lennard-Jones solid using multidimensional transition-state theory’’ *J. Chem. Phys.* **1998**, *109*, 8573-8582.

56. Reis, H.; Raptis, S.; Papadopoulos, M.G.; Janssen, R.H.C.; Theodorou, D.N.; Munn, R.W. ‘‘Calculation of macroscopic first and third-order optical susceptibilities for the benzene crystal’’ *Theor. Chem.Acc.* **1998**, *99*, 384-390.

57. Boulougouris, G.C.; Economou, I.G.; Theodorou, D.N. ‘‘On the Calculation of the Chemical

Potential Using the Particle Deletion Scheme'' *Molec. Phys.* **1999**, *96*, 905-913.

58. Spyriouni, T.; Economou, I.G.; Theodorou, D.N. ''Molecular Simulation of α-Olefins Using a New United Atom Potential: Vapor-Liquid Equilibria of Pure Compounds and Mixtures'' *J.Am.Chem.Soc.* **1999**, *121*, 3407-3413.

59. Gergidis, L.N.; Theodorou, D.N. ''Molecular dynamics simulation of *n*-butane - methane mixtures in silicalite'' *J. Phys. Chem. B* **1999**, *103*, 3380-3390.

60. Mavrantzas, V.G.; Boone, T.D.; Zervopoulou, E.; Theodorou, D.N. ''End-Bridging Monte Carlo: A Fast Algorithm for Atomistic Simulation of Condensed Phases of Long Polymer Chains'' *Macromolecules* **1999**, *32*, 5072-5096.

61. Mavrantzas, V.G.; Theodorou, D.N. ''Atomistic Simulation of the Birefringence of Uniaxially Stretched Polyethylene Melts'' *Comp.Theor.Polym.Sci.* **2000**, *10*, 1-13.

62. Gaub, M.; Fritzsche, S.; Haberlandt, R.; Theodorou, D.N. ''Van Hove Function for Diffusion in Zeolites'' *J. Phys. Chem. B* **1999**, *103*, 4721-4729.

63. Antoniadis, S.J.; Samara, C.T.; Theodorou, D.N. ''Effect of Tacticity on the Molecular Dynamics of Polypropylene Melts'' *Macromolecules* **1999**, *32*, 8635-8644.

64. Janssen, J.H.C.; Theodorou, D.N.; Raptis, S.; Papadopoulos, M.G. ''Molecular Simulation of Static hyper-Rayleigh Scattering: A Calculation of the Depolarization Ratio and the Local Fields for Liquid Nitrobenzene'' *J. Chem. Phys*. **1999**, *111*, 9711-9719.

65. Terzis, A.F.; Theodorou, D.N., Stroeks, A. ''Entanglement Network of the Polypropylene/Polyamide Interface. 1. Self-Consistent Field Model'' *Macromolecules* **2000**, *33*, 1385-1396.

66. Terzis, A.F.; Theodorou, D.N.; Stroeks, A. ''Entanglement Network of the Polypropylene/Polyamide Interface. 2. Network Generation'' *Macromolecules* **2000**, *33*, 1397-1410.

67. Doxastakis, M.; Kitsiou, M.; Fytas, G.; Theodorou, D.N.; Hadjichristidis, N.; Meier, G.; Frick, B. ''Component Segmental Mobility in an Athermal Polymer Blend: Quasielastic Incoherent Neutron Scattering vs Simulation'' *J. Chem. Phys.* **2000**, *112*, 8687-8694.

68. Gergidis, L.N.; Theodorou, D.N.; Jobic, H. ''Dynamics of *n*-butane-methane mixtures in silicalite using quasielastic meutron scattering and molecular dynamics simulations'' *J. Phys. Chem. B* **2000**, *104*, 5541-5552.

69. Harmandaris, V.A.; Mavrantzas, V.G.; Theodorou, D.N. ''Atomistic Molecular Dynamics Simulation of Stress Relaxation Upon Cessation of Steady-State Elongational Flow'' *Macromolecules* **2000**, *33*, 8062-8076.

70. Boulougouris, G.C.; Errington, J.R.; Economou, I.G.; Panagiotopoulos, A.Z.; Theodorou, D.N. ''Molecular Simulation of Phase Equilibria for Water – n-Butane and Water – n-Hexane Mixtures'' *J. Phys. Chem.B* **2000**, *104*, 4958-4963.

71. Karayiannis, N. Ch.; Mavrantzas, V.G.; Theodorou, D.N. ‘‘Diffusion of small molecules in disordered media: Study of the effect of kinetic and spatial heterogeneities’’ *Chem. Eng. Sci.* **2001**, *56*, 2789-2801.

72. Mavrantzas, V.G.; Theodorou, D.N. ‘‘Atomistic Monte Carlo simulation of steady-state uniaxial elongational flow of long-chain polyethylene melts: Dependence of the melt degree of orientation on stress, molecular length and elongational strain rate’’ *Macromol. Theory Simul.* **2000**, *9*, 500-515.

73. Reis, H.; Papadopoulos, M.G.; Theodorou, D.N. ‘‘Calculation of the refractive indices and third-harmonic generation susceptibilities of liquid benzene and water: Comparison of continuum and discrete local-field theories’’ *J. Chem. Phys.* **2001**, *114*, 876-881.

74. Makrodimitris, K.; Papadopoulos, G.K.; Theodorou, D.N. ‘‘Prediction of Permeation Properties of CO_2 and N_2 through Silicalite via Molecular Simulations’’ *J. Phys. Chem. B* **2001**, *105*, 777-788.

75. Faller, R.; Müller-Plathe, F.; Doxastakis, M.; Theodorou, D. ‘‘Local Structure and Dynamics in Trans-Polyisoprene Oligomers’’ *Macromolecules* **2001**, *34*, 1436-1448.

76. Zervopoulou, E.; Mavrantzas, V.G.; Theodorou, D.N. “A new Monte Carlo simulation approach for the prediction of sorption equilibria of oligomers in polymer melts: Solubility of long alkanes in linear polyethylene” *J. Chem. Phys.* **2001**, *115*, 2860-2875.

77. Boulougouris, G.C.; Voutsas, E.C.; Economou, I.G.; Theodorou, D.N.; Tassios, D.P. “Henry’s Constant Analysis for Water and Nonpolar Solvents from Experimental Data, Macroscopic Models, and Molecular Simulation” *J. Phys. Chem. B* **2001**, *105*, 7792-7798.

78. Rabias, I.; Langlois, C.; Provata, A.; Howlin, B.J.; Theodorou, D.N. “Linking the atomistic scale and the mesoscale: molecular orbital and solid state packing calculations on poly(p-phenylene)” *Polymer* **2002**, *43*, 185-193.

79. Boulougouris, G.C.; Economou, I.G.; Theodorou, D.N. “Calculation of the chemical potential of chain molecules using the staged particle deletion scheme” *J. Chem. Phys*. **2001**, *115*, 8231-8237.

80. Doxastakis, M.; Mavrantzas, V.G.; Theodorou, D.N. “Atomistic Monte Carlo simulation of *cis*-1,4 polyisoprene melts I. Single temperature end-bridging Monte Carlo simulations” *J. Chem. Phys*. **2001**, *115*, 11339-11351.

81. Doxastakis, M.; Mavrantzas, V.G.; Theodorou, D.N. “Atomistic Monte Carlo simulation of *cis*-1,4 polyisoprene melts II. Parallel tempering end-bridging Monte Carlo simulations” *J. Chem. Phys*. **2001**, *115*, 11352-11361.

82. Harmandaris, V.A.; Doxastakis, M.; Mavrantzas, V.G.; Theodorou, D.N. “Detailed molecular dynamics simulation of the self-diffusion of n-alkane and *cis*-1,4 polyisoprene oligomer melts” *J. Chem. Phys*. **2002**, *116*, 436-446.

83. Greenfield, M.L.; Theodorou, D.N. "Coarse-Grained Molecular Simulation of Penetrant Diffusion in a Glassy Polymer Using Reverse and Kinetic Monte Carlo" *Macromolecules* **2001**, *34*, 8541-8553.

84. Terzis, A.F.; Theodorou, D.N.; Stroeks, A. "Entanglement Network of the Polypropylene/Polyamide Interface 3. Deformation to Fracture" *Macromolecules* **2002**, *35*, 508-521.

85. Uhlherr, A.; Mavrantzas, V.G.; Doxastakis, M.; Theodorou, D.N. "Directed Bridging Methods for Atomistic Monte Carlo Simulations of Bulk Polymers" *Macromolecules* **2001**, 34, 8554-8568.

86. Uhlherr, A.; Doxastakis, M.; Mavrantzas, V.G.; Theodorou, D.N.; Leak, S.J.; Adam, N.E.; Nyberg, P.E. "Atomic structure of a high polymer melt" *Europhys. Lett*. **2002**, *57*, 506-511.

87. Uhlherr, A.; Leak, S.J.; Adam, N.E.; Nyberg, P.E.; Doxastakis, M.; Mavrantzas, V.G.; Theodorou, D.N. "Large scale atomistic polymer simulations using Monte Carlo methods for parallel vector processors" *Comput. Phys. Commun*. **2002**, *144*, 1-22.

88. Karayiannis, N.Ch.; Mavrantzas, V.G.; Theodorou, D.N. "A novel Monte Carlo scheme for the rapid equilibration of atomistic model polymer systems of precisely defined molecular architecture" *Phys. Rev. Lett*. **2002**, *88*, 105503.

89. Retsos, H.; Terzis, A.F.; Anastasiadis, S.H.; Anastassopoulos, D.L.; Toprakcioglu, C.; Theodorou, D.N.; Smith, G.S.; Menelle, A.; Gill, R.E.; Hadziioannou, G.; Gallot, Y. "Mushrooms and Brushes in Thin Films of Diblock Copolymer/Homopolymer Mixtures" *Macromolecules* **2002**, *35*, 1116-1132.

90. Harmandaris, V.A.; Angelopoulou, D.; Mavrantzas, V.G. ; Theodorou, D.N. "Atomistic molecular dynamics simulation of diffusion in binary liquid *n*-alkane mixtures" *J. Chem. Phys.* **2002**, *116*, 7656-7665.

91. Ahumada, O. ; Theodorou, D.N. ; Triolo, A.; Arrighi, V.; Karatasos, C.; Ryckaert, J.-P. "Segmental dynamics of atactic polypropylene as revealed by molecular simulations and quasielastic neutron scattering" *Macromolecules* **2002**, *35*, 7110-7124.

92. Karayiannis, N.Ch.; Giannousaki, A.E.; Mavrantzas, V.G.; Theodorou, D.N. ''Atomistic Monte Carlo of strictly monodisperse polyethylene melts through a generalized chain bridging algorithm'' *J. Chem. Phys.* **2002**, *117*, 5465-5479.

93. Makrodimitris, K.; Papadopoulos, G.K.; Philippopoulos, C.; Theodorou, D.N. "Parallel tempering method for reconstructing isotropic and anisotropic porous media" *J. Chem. Phys.* **2002**, *117*, 5876-5884.

94. Harmandaris, V.A.; Mavrantzas, V.G.; Theodorou, D.N.; Kröger, M.; Ramírez, J.; Öttinger, H.C.; Vlassopoulos, D. **''**Crossover from the Rouse to the entangled polymer melt regime: Signals from long, detailed atomistic molecular dynamics simulations, supported by rheological experiments'' *Macromolecules* **2003**, *36*, 1376-1387.

95. Arialdi, G., Ryckaert, J.-P.; Theodorou, D.N. "On the separation between torsion-vibration and conformational relaxation processes in the incoherent intermediate scattering function of polyethylene" *Chem. Phys*. **2003**, *292*, 371-382.

96. Doxastakis, M.; Theodorou, D.N.; Fytas, G.; Kremer, F.; Faller, R.; Müller-Plathe, F.; Hadjichristidis, N. "Chain and local dynamics of polyisoprene as probed by experiments and computer simulations'' *J. Chem. Phys.* **2003**, *119*, 6883-6894.

97. Gestoso, P.; Nicol, E.; Doxastakis, M.; Theodorou, D.N. "Atomistic Monte Carlo simulation of polybutadiene isomers: *cis*-1,4-polybutadiene and 1,2-polybutadiene'' *Macromolecules* **2003**, *36*, 6925-6938.

98. Eilmes, A.; Munn, R.W.; Mavrantzas, V.G.; Theodorou, D.N.; Góra, A. "Microscopic Calculation of the static electric susceptibility of polyethylene'' *J. Chem. Phys.* **2003**, *119*, 11458-11466.

99. Raptis, V.E.; Economou, I.G.; Theodorou, D.N.; Petrou, J.; Petropoulos, J.H. "Molecular dynamics simulation of structure and thermodynamic properties of poly(dimethylsilamethylene) and hydrocarbon solubility therein: Towards the development of novel membrane materials for hydrocarbon separation'' *Macromolecules* **2004**, *37*, 1102-1112.

100. Daoulas, K. Ch.; Theodorou, D.N.; Roos, A.; Creton, C. "Experimental and self-consistent field theoretical study of styrene block copolymer self-adhesive materials" *Macromolecules* **2004**, *37*, 5093-5109.

101. Karayiannis, K. Ch.; Mavrantzas, V.G.; Theodorou, D.N. "Detailed atomistic simulation of the segmental dynamics and barrier properties of amorphous poly(ethylene terephthalate) and poly(ethylene isophthalate)" *Macromolecules* **2004**, *37*, 2978-2995.

102. Papadopoulos, G.K.; Jobic, H.; Theodorou, D.N. "Transport diffusivity of N_2 and CO_2 in silicalite: Coherent quasielastic neutron scattering measurements and molecular dynamics simulations" *J. Phys. Chem. B* **2004**, *108*, 12748-12756.

103. Wick, C.D. and Theodorou, D.N. "Connectivity-altering Monte Carlo simulations of the end group effects on volumetric properties of poly(ethylene oxide)" *Macromolecules* **2004**, *37*, 7026-7033.

104. Peristeras, L.D.; Economou, E.G.; Theodorou, D.N. "Structure and volumetric properties of linear and triarm star polyethylenes from atomistic Monte Carlo simulation using new internal rearrangement moves" *Macromolecules* **2005**, *38*, 386-397.

105. Tsolou, G.; Mavrantzas, V.G.; Theodorou, D.N. "Detailed atomistic molecular dynamics simulation of cis-1,4 polybutadiene" *Macromolecules* **2005**, *38*, 1478-1492.

106. Daoulas, K.Ch.; Theodorou, D.N.; Harmandaris, V.A.; Karayiannis, N. Ch.; Mavrantzas, V.G. "Self-consistent field study of compressible, semi-flexible melts, adsorbed on a solid substrate and comparison with atomistic simulations" *Macromolecules* **2005**, *38*, 7134-7149.

107. Kortunov, P.; Vasenkov, S.; Kärger, J.; Elía, M.F.; Perez, M., Stöcker, M.; Papadopoulos, G.K.; Theodorou, D.; Drescher, B.; McElhiney, G.; Bernauer, B.; Krystl, V.; Kočiřik, M.; Zikánová, A.; Jirglová, H.; Berger, C.; Gläser, R.; Weitkamp, J.; Hansen, E.W. "Diffusion in fluid catalytic cracking catalysts on various displacement scales and its role in catalytic performance" *Chem. Mater*. **2005**, *17*, 2466-2474.

108. Economou, I.G.; Raptis, V.E.; Melissas, V.S.; Theodorou, D.N., Petrou, J.; Petropoulos, J.H. "Molecular simulation of structure, thermodynamic and transport properties of polymeric membrane materials for hydrocarbon separation" *Fluid Phase Equilibria* **2005**, *228-229*, 15-20.

109. Kortunov, P.; Vasenkov, S.; Kärger, J.; Elía, M.F.; Perez, M., Stöcker, M.; Papadopoulos, G.K.; Theodorou, D.; Drescher, B.; McElhiney, G.; Bernauer, B.; Krystl, V.; Kočiřik, M.; Zikánová, A.; Jirglová, H.; Berger, C.; Gläser, R.; Weitkamp, J.; Hansen, E.W. "Pulsed-field gradient nuclear magnetic resonance study of transport properties of fluid catalytic cracking catalysts" *Magn. Reson. Imaging* **2005**, *23*, 233-237.

110. Zacharopoulos, N.; Vergadou, N.; Theodorou, D.N. "Coarse-graining using pre-tabulated potentials: Liquid benzene" *J. Chem. Phys.* **2005**, *122*, 244111.

111. Wick, C.D.; Siepmann, J.I.; Theodorou, D.N. "Microscopic origins for the favorable solvation of carbonate ether copolymers in CO_2" *J. Am. Chem. Soc*. **2005**, *127*, 12338-12342.

112. Theodorou, D.N. "A reversible minimum-to-minimum mapping method for the calculation of free-energy differences" *J. Chem. Phys.* **2006**, *124*, 034109.

113. Jobic, H. and Theodorou, D.N. "Diffusion of long n-alkanes in silicalite. A comparison between neutron scattering experiments and hierarchical simulation results" *J. Phys. Chem. B* **2006**, *110*, 1964-1967.

114. Tzoumanekas, C.; Theodorou, D.N. "Topological analysis of linear polymer melts: A statistical approach" *Macromolecules* **2006**, *39*, 4592-4603.

115. Uhlherr, A.; Theodorou, D.N. "Accelerating molecular simulations by reversible mapping between local minima" *J. Chem. Phys*. **2006**, *125*, 084107.

116. Leyssale, J.-M.; Papadopoulos, G.K.; Theodorou, D.N. "Sorption thermodynamics of CO_2, N_2, and their mixtures in the ITQ-1 zeolite as revealed by molecular simulations" *J. Phys. Chem. B* **2006**, *110*, 22742-22753.

117. Kamio, K.; Moorthi, K.; Theodorou, D.N. "Coarse-grained end bridging Monte Carlo simulations of poly(ethylene terephthalate) melt" *Macromolecules* **2007**, *40*, 710-722.

118. Rabias, I.; Howlin, B.J.; Provata, A.; Theodorou, D.N. "Modeling of structural and vibrational properties of poly(p-phenylene) and polypyrrole using molecular orbital methods" *Molecular Simulation* **2000**, *24*, 95.

119. Logotheti, G.E.; Theodorou, D.N. "Segmental and chain dynamics of isotactic polypropylene melts" *Macromolecules* **2007**, *40*, 2235-2245.

120. Papadopoulos, G.K.; Theodorou, D.N.; Vasenkov, S.; Kärger, J. "Mesoscopic simulations of the diffusivity of ethane in beds of NaX zeolite crystals: Comparison with pulsed field gradient NMR measurements" *J.Chem.Phys.* **2007**, *126*, 094702.

121. Peristeras, L.D.; Rissanou, A.N.; Economou, I.G.; Theodorou, D.N. "Novel Monte Carlo molecular simulation scheme using identity-altering elementary moves for the calculation of structure and thermodynamic properties of polyolefin blends" *Macromolecules* **2007**, *40*, 2904-2914.

122. Spyriouni, T.; Tzoumanekas, C.; Theodorou, D.; Müller-Plathe, F.; Milano, G. "Coarse-grained and reverse-mapped united-atom simulations of long-chain atactic polystyrene melts: structure, thermodynamic properties, chain conformation, and entanglements" *Macromolecules* **2007**, *40*, 3876-3885.

123. Johansson, E.; Bolton, K.; Theodorou, D.N.; Ahlström, P. "Monte Carlo simulations of equilibrium solubilities and structure of water in n-alkanes and polyethylene" *J. Chem. Phys.* **2007**, 126, 224902.

124. Boulougouris, G.C.; Theodorou, D.N. "Dynamical Integration of a Markovian Web: A first passage time approach" *J. Chem. Phys.* **2007**, 127, 084903.

125. Johansson, E.; Bolton, K.; Theodorou, D.N.; Ahlström, P. "Formation of rodlike structures of water between oppositely charged ions in decane and polyethylene" *J. Chem. Phys.* **2007**, *127*, 191101.

126. Sant, M.; Papadopoulos, G.K.; Theodorou, D.N. "A second-order Markov process for modeling diffusion through spatial discretization" *J. Chem. Phys.* **2008**, *128*, 024504.

127. Ramos, J.; Peristeras, L.D.; Theodorou, D.N. "Monte Carlo Simulation of Short Chain Branched Polyolefins in the Molten State" *Macromolecules* **2007**, *40*, 9640-9650.

128. Ramos, J.; Vega, J.F.; Theodorou, D.N. "Entanglement relaxation time in polyethylene: Simulation versus experimental data" *Macromolecules* **2008**, *41*, 2959-2962.

129. Tsalikis, D.G.; Lempesis, N.; Boulougouris, G.C.; Theodorou, D.N. "On the role of inherent structures in glass-forming materials I. The vitrification process" *J. Phys. Chem. B* **2008**, *112*, 10619-10627.

130. Tsalikis, D.G.; Lempesis, N.; Boulougouris, G.C.; Theodorou, D.N. "On the role of inherent structures in glass-forming materials II. Reconstruction of the mean square displacement by rigorous lifting of the inherent structure dynamics" *J. Phys. Chem. B* **2008**, *112*, 10628-10637.

131. Pantatosaki, E.; Jobic, H.; Papadopoulos, G.K.; Theodorou, D.N. "Combined atomistic simulation and quasielastic neutron scattering study of the low-temperature dynamics of hydrogen and deuterium confined in NaX zeolite" *J. Phys. Chem. B* **2008**, *112*, 11708-11715.

132. Papadopoulos, G.K.; Theodorou, D.N. "Simulation studies of methane, carbon dioxide, hydrogen, and deuterium in ITQ-1 and NaX zeolites" *Molecular Simulation* **2009**, *35*, 79-89.

133. Spyriouni, T.; Boulougouris, G.C.; Theodorou, D.N. “Prediction of sorption of CO_2 in glassy atactic polystyrene at elevated pressures through a new computational scheme” *Macromolecules* **2009**, *42*, 1759-1769.

134. Boulougouris, G.C.; Theodorou, D.N. “Probing subglass relaxation in polymers via a geometric representation of probabilities, observables, and relaxation modes in discrete stochastic systems” *J. Chem. Phys*. **2009**, *130*, 044905.

135. Sant, M.; Leyssale, J.-M.; Papadopoulos, G.K. ; Theodorou. D.N. “Molecular dynamics of carbon dioxide, methane and their mixtures in a zeolite possessing two independent pore networks as revealed by computer simulations” *J. Phys. Chem. B* **2009**, *113*, 13761-13767.

136. Tzoumanekas, C.; Lahmar, F.; Rousseau, B.; Theodorou, D.N. “Onset of entanglements revisited. Topological analysis” *Macromolecules* **2009**, *42*, 7474-7484.

137. Lahmar, F.; Tzoumanekas, C.; Theodorou, D.N.; Rousseau, B. “Onset of entanglements revisited. Dynamical analysis” *Macromolecules* **2009**, *42*, 7485-7494.

138. Megariotis, G.; Vyrkou, A.; Leygue, A.; Theodorou, D.N. “Systematic coarse-graining of 4-cyano-4′-pentylbiphenyl” *Ind. Eng. Chem*. **2011,** *50*, 546-556.

139. Sant, M.; Papadopoulos, G.K.; Theodorou, D.N. “Diffusion via space discretization method to study the concentration dependence of self-diffusivity under confinement” *J. Chem. Phys.* **2010**, *132*, 134108.

140. Tsalikis, D.G.; Lempesis, N.; Boulougouris, G.C.; Theodorou, D.N. “Efficient parallel decomposition of dynamical sampling in glass-forming materials based on an “on-the-fly” definition of metabasins” *J. Chem. Theory Comput.* **2010**, *6*, 1307-1322.

141. De Angelis, M.G.; Boulougouris, G.C.; Theodorou, D.N. “Prediction of infinite dilution benzene solubility in linear polyethylene melts via the Direct Particle Deletion method” *J. Phys. Chem. B* **2010**, *114*, 6233-6246.

142. Tsalikis, D.G.; Lempesis, N.; Boulougouris, G.C.; Theodorou, D.N. “Temperature-accelerated dynamics in glass-forming materials” *J. Phys. Chem. B* **2010**, *114*, 7844-7863.

143. Romanos, N.A.; Theodorou, D.N. “Crystallization and melting simulations of oligomeric α1 isotactic polypropylene” *Macromolecules* **2010**, *43*, 5455-5469.

144. Boulougouris, G.C.; Peristeras, L. ; Economou, I.G. ; Theodorou, D.N. “Predicting phase equilibrium via histogram reweighting with Gibbs ensemble Monte Carlo simulations” *J. of Supercritical Fluids* **2010**, *55*, 503-509.

145. Vogiatzis, G.G.; Voyiatzis, E.; Theodorou, D.N. “Monte Carlo simulations of a coarse-grained model for an athermal all-polystyrene nanocomposite system” *Eur. Polym. J*. **2011**, *47*, 699-712.

146. Ndoro, T.M.; Voyiatzis, E.; Ghanbari, A.; Theodorou, D.N.; Böhm, M.; Müller-Plathe, F. "Interface of grafted and ungrafted silica nanoparticles with a polystyrene matrix: Atomistic Molecular Dynamics simulations" *Macromolecules* **2011**, *44*, 2316-2327.

147. Panagiotou, E.; Tzoumanekas, C.; Lambropoulou, S.; Millett, K.C.; Theodorou, D.N. "A Study of the entanglement in systems with periodic boundary conditions" *Prog. Theor. Phys. Suppl*. **2011**, *191*, 172-181.

148. Lempesis, N.; Tsalikis, D.G.; Boulougouris, G.C.; Theodorou, D.N. "Lumping analysis for the prediction of long-time dynamics: From monomolecular reaction systems to inherent structure dynamics in glassy materials" *J. Chem. Phys*. **2011**, *135*, 204507.

149. Kolokathis, P.D.; Theodorou, D.N. "On solving the master equation in spatially periodic systems" *J. Chem. Phys*. **2012**, *137*, 034112.

150. Moorthi, K.; Kamio, K.; Ramos, J.; Theodorou, D.N. "Monte Carlo simulation of short-chain branched polyolefins: Structure and Properties" *Macromolecules* **2012**, *45*, 8453-8466.

151. Anogiannakis, S.; Tzoumanekas, C.; Theodorou, D.N. "Microscopic description of entanglements in polyethylene networks and melts: Strong, weak, pairwise, and collective attributes" *Macromolecules* **2012**, *45*, 9475-9492.

152. Lempesis, N.; Boulougouris, G.C.; Theodorou, D.N. "Temporal disconnectivity of the energy landscape in glassy systems" *J. Chem. Phys*. **2013**, *138*, 12A545.

153. Vogiatzis, G.G.; Theodorou, D.N. "Structure of polymer layers grafted to nanoparticles in silica-polystyrene nanocomposites" *Macromolecules* **2013**, *46*, 4670-4683.

154. Morozinis, A.K.; Tzoumanekas, C.; Anogiannakis, S.D.; Theodorou, D.N. "Atomistic simulations of cavitation in a model polyethylene network" *Polym. Sci. – Ser. C* **2013**, *55*, 212-218.

155. Lempesis, N.; Vogiatzis, G.G.; Boulougouris, G.C.; van Breemen, L.C.A.; Hütter, M.; Theodorou, D.N. "Tracking a glassy polymer on its energy landscape in the course of elastic deformation" *Mol. Phys*. **2013**, *111*, 3430-3441.

156. Kolokathis, P.D.; Pantatosaki, E.; Gatsiou, C.-A.; Jobic, H.; Papadopoulos, G.K.; Theodorou, D.N. "Dimensionality reduction of free energy profiles of benzene in silicalite-1: calculation of diffusion coefficients using transition state theory" *Molec. Simul*. **2013**, *40*, 80-100.

157. Vogiatzis, G.G.; Theodorou, D.N. "Local segmental dynamics and stresses in polystyrene-C_{60} mixtures" *Macromolecules* **2014**, *47*, 387-404.

158. Theodorou, D.N.; Vogiatzis, G.G.; Kritikos, G. "Self-consistent field study of adsorption and desorption kinetics of polyethylene melts on graphite and comparison with atomistic simulations" *Macromolecules* **2014**, *47*, 6964-6981.

159. Moorthi, K.; Kamio, K.; Ramos, J.; Theodorou, D.N. "Monte Carlo simulations of structure and entanglements in polymer melts" *Molecular Simulation* **2014**, *41*, 993-995.

160. Skountzos, E. N.; Anastasiou, A.; Mavrantzas, V.G.; Theodorou, D.N. "Determination of the mechanical properties of a poly(methyl methacrylate) nanocomposite with functionalized graphene sheets through atomistic simulations" *Macromolecules* **2014**, *47*, 8072-8088.

161. Ziogos, O.G.; Theodorou, D.N. "Molecular dynamics simulations of alkyl substituted nanographene crystals" *Molec. Phys*. **2015**, *113*, 2776-2790.

162. Mathioudakis, I.G.; Vogiatzis, G.G.; Tzoumanekas, C.; Theodorou, D.N. "Molecular modeling and simulation of polymer nanocomposites at multiple length scales" *IEEE Trans. on Nanotech.* **2016**, *15*, 416-422.

163. Romanos, N.A.; Theodorou, D.N. "Melting point and solid-liquid coexistence properties of α_1 isotactic polypropylene as functions of its molar mass: A molecular dynamics study" *Macromolecules* **2016**, *49*, 4663-4673.

164. Kolokathis, P.D.; Kali, G.; Jobic, H.; Theodorou, D.N. "Diffusion of aromatics in silicalite-1: Experimental and Theoretical Evidence for Entropic Barriers" *J. Phys. Chem. C* **2016**, *120*, 21410-21426.

165. Mathioudakis, I.G.; Vogiatzis, G.G.; Tzoumanekas, C,; Theodorou, D.N. "Multiscale simulations of PS-SiO_2 nanocomposites: from melt to glassy state" *Soft Matter* **2016**, *12*, 7585-7605.

167. Vogiatzis, G.G.; Megariotis, G.; Theodorou, D.N. "Equation of state based slip spring model for entangled polymer dynamics" *Macromolecules* **2017**, *50*, 3004-3029.

168. Liossi, A.S.; Ntountaniotis, D.; Kellici, T.F.; Chatziathanasiadou, M.V.; Megariotis, G.; Mania, M.; Becker-Baldus, J.; Kriechbaum, M.; Krajnk, A.; Christodoulou, E.; Glaubitz, C.; Rappolt, M.; Amenitsch, H.; Mali, G.; Theodorou, D.N.; Valsami, G.; Pitsikalis, M.; Iatrou, H.; Tzakos, A.; Mavromoustakos, Th. "Exploring the interactions of irbesartan and rbesartan-2-isopropyl β-cyclodextrin complex and irbesartan-2-cyclopropene with model membranes" *Biochim. Biophys. Acta* **2017**, *1859*, 1089-1098.

169. Tzounis, P.-N.; Anogiannakis, S.; Theodorou, D.N. "General methodology for estimating the stiffness of polymer chains from their chemical constitution: A single unperturbed chain Monte Carlo Algorithm" *Macromolecules* **2017**, *50*, 4575-4587.

170. Sgouros, A.P.; Megariotis, G.; Theodorou, D.N. "Slip-spring model for the linear and nonlinear viscoelastic properties of molten polyethylene derived from atomistic simulations" *Macromolecules* **2017**, *50*, 4524-4541.

171. Sgouros, A.P.; Vogiatzis, G.G.; Kritikos, G.; Boziki, A.; Nikolakopoulou, A.; Liveris, D.; Theodorou, D.N. "Molecular simulations of free and graphite capped polyethylene films: Estimation of the interfacial free energies" *Macromolecules* **2017**, *50*, 8827-8844.

172. Galata, A.A.; Anogiannakis, S.D.; Theodorou, D.N. "Thermodynamic analysis of Lennard-Jones binary mixtures using Kirkwood-Buff theory" *Fluid Phase Equilibria* **2018**, *470*, 25-37.

173. Ziogos, O.G.; Konstantinopoulos, S.; Tsetseris, L.; Theodorou, D.N. "Computational studies of nanographene systems: Extended discotics, covalently linked 'Supermolecules,' and functionalized supramolecular assemblies" *J. Phys. Chem. C* **2018**, *122*, 18715-18731.

174. Tzounis, P.-N.; Argyropoulou, D.V.; Anogiannakis, S.D.; Theodorou, D.N. "Tacticity effect on the conformational properties of polypropylene and poly(ethylene-propylene) copolymers" *Macromolecules* **2018**, 51, 6878-6891.

175. Megariotis, G.; Vogiatzis, G.G.; Sgouros, A.P.; Theodorou, D.N. "Slip-Spring Based Mesoscopic Simulations of Polymer Networks: Methodology and the Corresponding Computational Code" *Polymers* **2018**, *10*, 1156.

176. Sgouros, A.P.; Lakkas, A.T.; Megariotis, G.; Theodorou, D.N. "Mesoscopic Simulations of Free Surfaces of Molten Polyethylene: Brownian Dynamics/Kinetic Monte Carlo Coupled with Square Gradient Theory and Compared to Atomistic Calculations and Experiment" *Macromolecules* **2018**, *51*, 9798-9815.

177. Chatzieleftheriou, S.; Anogiannakis, S.; Theodorou, D.N.; Lagaros, N.D. "SIMNANO: A Trust Region Strategy for Large Scale Molecular Systems Energy Minimization Based on Exact 2nd Order Derivative Information". *J. Chem. Inf. Model.* **2019**, 59, 190-205.

178. Petris, P. C.; Anogiannakis, S.D.; Tzounis, P.-N.; Theodorou, D.N. "Thermodynamic Analysis of n-Hexane/Ethanol Binary Mixtures Using Kirkwood-Buff Theory". *J. Phys. Chem. B*. **2019**, *123*, 247-257.

179. Kallivokas, S.V.; Sgouros, A.P.; Theodorou, D.N. "Molecular Dynamics Simulations of EPON-862/DETDA Epoxy Networks: Structure, Topology, Elastic Constants, and Local Dynamics". *Soft Matter* **2019**, *15*, 721-733.

180. Lakkas, A.T.; Sgouros, A.P.; Theodorou, D.N. "Self-Consistent Field Theory Coupled with Square Gradient Theory of Free Surfaces of Molten Polymers and Compared to Atomistic Simulations and Experiment" *Macromolecules* **2019**, *52*, 5337-5356.

181. Sgouros, A.P.; Vogiatzis, G.G.; Megariotis, G.; Tzoumanekas, C.; Theodorou, D.N. "Multiscale simulations of graphite-capped polyethylene melts: Brownian dynamics/kinetic Monte Carlo compared to atomistic simulations and experiment" *Macromolecules* **2019**, *52*, 7503-7523.

182. Anogiannakis, S.D.; Petris, P.C.; Theodorou, D.N. "A Promising Route for the Development of a Computational Framework for Self-Assembly and Phase Behavior Prediction of Ionic Surfactants Using MARTINI" *J. Phys. Chem. B* **2019**, *52*, 7503-7623.

183. Sgouros, A.P.; Theodorou, D.N. "Atomistic simulations of long-chain polyethylene melts flowing past gold surfaces: structure and wall-slip" *Molec. Phys*. **2020**, *118*, e1706775.

184. Nieto Simavilla, D.; Sgouros, A.P.; Vogiatzis, G.G.; Tzoumanekas, C.; Georgilas, V.; Verbeeten, W. M. H.; Theodorou, D.N. "Molecular Dynamics Test of the Stress-Thermal Rule in Polyethylene and Polystyrene Melts" *Macromolecules* **2020**, *53*, 789-802

185. Vogiatzis, G.G.; Van Breemen, L.C.A.; Theodorou, D.N.; Hütter, M. “Free energy calculations by molecular simulations of deformed polymer glasses” *Comp. Phys. Commun.* **2020**, *249*, 107008.

186. Ricci, E.; Vergadou, N.; Vogiatzis, G.G.; De Angelis, M.G.; Theodorou, D.N. “Molecular Simulations and Mechanistic Analysis of the Effect of CO_2 Sorption on Thermodynamics, Structure, and Local Dynamics of Molten Atactic Polystyrene” *Macromolecules* **2020**, *53*, 3669-3689.

187. Kallivokas, S.V.; Sgouros, A.P.; Theodorou, D.N. “Kinetic concepts and local failure in the interfacial shear strength of epoxy-graphene nanocomposites” *Phys. Rev. E* **2020**, *102*, 030501.

188. Romanos, N.; Megariotis, G.; Theodorou, D.N. “Molecular dynamics simulations of stretch-induced crystallization in layered polyethylene” *Polymer Crystallization* **2021**, *4*, e10172.

189. Lakkas, A.T.; Sgouros, A.P.; Revelas, C.J.; Theodorou, D.N. “Structure and thermodynamics of grafted silica/polystyrene dilute nanocomposites investigated through self-consistent field theory” *Soft Matter* **2021**, *17*, 4077-4097.

190. Sgouros, A.P.; Revelas, C.J.; Lakkas, A.T.; Theodorou, D.N. “Potential of Mean Force between Bare or Grafted Silica/Polystyrene Surfaces from Self-Consistent Field Theory” *Polymers* **2021**, *13*, 1197.

191. Sgouros, A.P.; Knippenberg, S.; Guillaume, M.; Theodorou, D.N. “Multiscale simulations of polyzwitterions in aqueous bulk solutions and brush array configurations” *Soft Matter* **2021**, *17*, 10873-10890.

192. Revelas, C.J.; Sgouros, A.P.; Lakkas, A.T.; Theodorou, D.N. “RuSseL: A Self-Consistent Field Theory Code for Inhomogeneous Polymer Interphases” *Computation* **2021**, *9*, 57.

193. Sgouros, A.P.; Tsagkalakis, D.; Theodorou, D.N. “Effect of Surface Nanopatterning on Slip: The Case of Couette Flow of Long-Chain Polyethylene Melt Flowing past Gold Surfaces” *J. Phys. Chem.* **2021**, *125*, 6681-6696.

194. Megariotis, G.; Romanos, N.; Avramopoulos, A.; Mikaelian, G.; Theodorou, D.N. “In silico study of levodopa in hydrated lipid bilayers at the atomistic level” *J. Mol. Graph. Model.* **2021**, *107*, 107972.

195. Sigalas, N.I.; Anogiannakis, S.A.; Theodorou, D.N.; Lyulin, A.V. “A coarse-grained model for capturing the helical behavior of isotactic polypropylene” *Soft Matter* **2022**, *18*, 3076-3086.

196. Venetsanos, F.; Anogiannakis, S.; Theodorou, D.N. “Mixing thermodynamics and Flory-Huggins interaction parameter of polyethylene oxide/polyethylene oligomeric blends from Kirkwood-Buff theory and molecular simulations” *Macromolecules* **2022**, *55*, 4852-4862.

197. Megariotis, G.; Mikaelian, G.; Avramopoulos, A.; Romanos, N.; Theodorou, D.N. "Molecular simulations of fluoxetine in lipid bilayers, as well as in aqueous solutions containing β-cyclodextrin" *J. Molec. Graph. Model.* **2022**, *117*, 108305.

198. Sgouros, A.P.; Revelas, C.J.; Lakkas, A.T.; Theodorou, D.N. "Solvation free energy of dilute grafted nanoparticles in polymer melts via self-consistent field theory" *J. Phys. Chem. B* **2022**, *126*, 7454-7474.

B. Book Chapters, Review Papers, Editorials

1. Mansfield, K.F.; Theodorou, D.N. "Molecular Mechanics Simulation of Glassy Polymers at Interfaces", in *Computer Simulation of Polymers*; Roe, R.-J., Ed; Prentice-Hall: Englewood Cliffs, 1991; pp 122-140.

2. Theodorou, D.N. "Molecular and Computer Modeling of Polymer Surfaces and Polymer/Solid Interfaces", in *Physics of Polymer Surfaces and Interfaces*; Sanchez, I.C., Ed; Butterworth-Heinemann, Boston and Manning, Greenwich, CT, 1992; pp 139-162.

3. Theodorou, D.N. "Modeling of Polymer Structure and Properties", in *Encyclopedia for Advanced Materials*; Bloor, D.; Brook, R.J.; Flemings, M.C.; Mahajan, S., Eds; Pergamon Press: Oxford, 1994.

4. Dodd, L.R.; Theodorou, D.N. "Atomistic Monte Carlo Simulation and Continuum Mean Field Theory of the Structure and Equation of State Properties of Alkane and Polymer Melts", in *Atomistic Modeling of Physical Properties*; Monnerie, L.M.; Suter, U.W., Eds.; Advances in Polymer Science No 116; Springer-Verlag: Berlin, 1994; pp 249-281.

5. Theodorou, D.N. "Molecular Simulations of Sorption and Diffusion in Amorphous Polymers", in *Diffusion in Polymers*; Neogi, P., Ed; Marcel Dekker, 1996; pp 67-142.

6. Theodorou, D.N. "Symposium in Print on Molecular Modeling", Editorial. *Chem.Eng.Sci.* **1994**, *49*, 2715-2716.

7. Theodorou, D.N.; Snurr, R.Q.; Bell, A.T. "Molecular Dynamics and Diffusion in Microporous Materials", in *Comprehensive Supramolecular Chemistry*, Volume 7; Alberti, G. and Bein, T., Eds; Elsevier Science: Oxford, 1996; pp 507-548.

8. Bell, A.T.; Maginn, E.J.; Theodorou, D.N. "Molecular Simulation of Adsorption and Diffusion in Zolites", in *Handbook of Heterogeneous Catalysis;* Ertl, G.; Knözinger, H.; Weitkamp, J., Eds; VCH: Weinheim, 1997; Vol. 3, pp 1165-1188.

9. Theodorou, D.N. ''Transition-state theory investigations of small molecule diffusion in glassy polymers'', in *Classical and Quantum Dynamics in Condensed Phase Simulations*; Berne, B.J.; Ciccotti, G.; Coker, D.F., Eds; World Scientific: Singapore, 1998; pp 211-249.

10. Uhlherr, A.; Theodorou, D.N. ''Hierarchical simulation approach to structure and dynamics of polymers'' *Current Opinion in Solid State and Materials Science* **1998**, *3*, 544-551.

11. Rutledge, G.C.; Theodorou, D.N. ‘‘Interdisciplinary Workshop on Molecular Modeling of Polymers,’’ Preface, *Macromol. Symp*. **1998**, *133*, 1-112

12. Theodorou, D.N. ‘‘Hierarchical Modeling of Polymers,’’ SIMU Program Newsletter, Issue 1, Spring 2000, p 19-40. *http://simu.ulb.ac.be/newsletters/newsletter.html*

13. Theodorou, D.N. “Variable Connectivity Monte Carlo Algorithms for the Atomistic Simulation of Long-Chain Polymer Systems”. In Nielaba, P. ; Mareschal, M. ;. Ciccotti, G. (editors), *Bridging Time Scales : Molecular Simulations for the Next Decade*; Lecture Notes in Physics **605**; Springer-Verlag : Berlin, 2002 ; pp 67-127.

14. Theodorou, D.N. “Polymers at Surfaces and Interfaces”, in *Computer Simulations of Surfaces and Interfaces*; Dünweg, B.; Landau, D.P.; Milchev, A., Eds.; Kluwer Academic Publishers (NATO Science Series II/114): Dordrecht, 2003; pp 329-419.

15. Theodorou, D.N. “Understanding and predicting structure-property relations in polymeric materials through molecular simulations’’ *Mol. Phys*. **2004**, *102*, 147-166.

16. Theodorou, D.N. “Multiscale Modeling of Polymers”, perspective 15 in *Handbook of Materials Modeling*. *Volume I: Methods and Models*; Yip, S., Ed.; Springer, 2005, pp 2757-2761.

17. Theodorou, D.N. “Principles of molecular simulation of gas transport in polymers”, in *Materials Science of Membranes for Gas and Vapor Separation*; Yampolskii, Yu.; Pinnau, I.; Freeman, B.D., Eds.; John Wiley: Hoboken, NJ, 2006; pp 49-94.

18. Theodorou, D.N. “Hierarchical modeling of amorphous polymers”, *Comp. Phys. Commun.* **2005**, *169*, 82-88.

19. Theodorou, D.N. “Equilibration and coarse-graining methods for polymers”, in *Computer Simulations in Condensed Matter: From Materials to Chemical Biology*; Lecture Notes in Physics; Ferrario, M., Ciccotti, G., Binder, K., Eds.; Springer: Berlin, 2006, pp 419-448.

20. Papadopoulos, G.K.; Theodorou, D.N. “Computer Simulation of Sorption and Transport in Zeolites”, in *Handbook of Heterogeneous Catalysis*, 2nd Edition; Ertl, G.; Knözinger, H.; Schüth, F.; Weitkamp, J.; Eds.; Wiley-VCH: Weinheim, 2008; Chapter 5.5.2, pp 1662-1676.

21. Tzoumanekas, C.; Theodorou, D.N. “From atomistic simulations to slip-link models of entangled polymer melts: Hierarchical strategies for the prediction of rheological properties”, *Current Opinion in Solid State and Materials Science* **2006**, *10*, 61-72.

22. Jobic, H.; Theodorou, D.N. “Quasi-elastic neutron scattering and molecular dynamics simulation as complementary techniques for studying diffusion in zeolites” *Microp. Mesop. Mater*. **2007**, *102*, 21-50.

23. Theodorou, D.N. “Hierarchical modeling of polymeric materials” *Chem. Eng. Sci*. **2007**, *62*, 5697-5714.

24. Stallmach, F.; Snurr, R.Q.; Stöcker, M.; Theodorou, D.N. “Diffusion in Micropores”, Editorial, *Microp. Mesop. Mater.* **2009**, *125*, 1-2.

25. Theodorou, D.N. “Progress and outlook in Monte Carlo Simulations” *Ind. Eng. Chem. Res*. **2010**, 49, 3047-3058.

26. Theodorou, D.N. “Tracking the Dynamics of Systems Evolving through Infrequent Transitions in a Network of Discrete States”, in *Hierarchical Methods for Dynamics in Complex Molecular Systems*; Grotendorst, J.; Sutmann, G; Gompper, G.; Marx, D.; Eds.; Schriften des Forschungzentrums Jülich, IAS Series Volume 10: Jülich, 2012; pp 347-389.

27. Biggs, M.J.; Theodorou, D.N. “2013 Danckwerts special issue on molecular modelling in chemical engineering” (Editorial), *Chem. Eng. Sci*. **2015**, *121*, 1-2.

28. Kärger, J; Caro, J.; Cool, P.; Coppens, M.-O.; Jones, D.; Kapteijn, F.; Rodriguez-Reinoso, F.; Stöcker, M.; Theodorou, D.; Vansant, E.F.; Weitkamp, J. “Benefit of microscopic diffusion measurement for the characterization of nanoporous materials” *Chem. Eng. Tech*. **2009**, *32*, 1494-1511.

29. Papadopoulos, K.G.; Theodorou, D.N. “Hierarchical simulations of diffusion in zeolites,” in *Diffusion Fundamentals : Leipzig 2005*, Kärger, J.; Grinberg, F.; Heitjans, P.; Eds.; Leipziger Universitätsverlag, 2005; pp 80-104.

30. Vogiatzis, G.G.; Theodorou, D.N. “Multiscale molecular simulations of polymer-matrix nanocomposites, or What molecular simulations have taught us about the fascinating nanoworld” *Arch. Computat. Methods Engin.* **2018**, 25, 591-645.

31. Vergadou, N.; Theodorou, D.N. “Molecular Modeling Investigations of Sorption and Diffusion of Small Molecules in Glassy Polymers” *Membranes* **2019**, *9*, 98.

32. Alexiadis, O.; Cheimarios, N.; Peristeras, L.D.; Bick, A.; Mavrantzas, V.G.; Theodorou, D.N.; Hill, J.-R.; Krokidis, X. “Chameleon: A generalized, connectivity-altering software for tackling the properties of realistic polymer systems” *Wiley Interdisciplinary Reviews: Computational Molecular Science* **2019**, *9*, e1414.

C. Textbooks

1. *Applied Molecular Theory for Chemical Engineers* (with Arup K. Chakraborty), a set of class notes, U.C. Berkeley, 1993.

2. *Physical Chemistry of Polymers*, a set of class notes, University of Patras, 1999 (in Greek).

3. *Simulation Methods for Polymers* (co-edited with Michael J. Kotelyanskii), Marcel Dekker, 2004, ISBN: 0-8247-0247-6

4. *Diffusion in Nanoporous Materials*, in 2 volumes (with Jörg Kärger and Douglas M. Ruthven), Wiley-VCH, 2012, ISBN: 978-3-527-31024-1

D. Conference Proceedings, Research Reports

1. Theodorou, D.N.; Suter, U.W. “Molecular Structure of a Vinyl Polymer Glass” *Polym.Prepr., Am.Chem.Soc., Div.Polym.Chem.* **1984**, *25*(1), 180.

2. Theodorou, D.N.; Suter, U.W. “Local Structure and the Response of a Polymeric Glass to Elastic Deformation” *Polym.Prepr., Am. Chem. Soc., Div. Polym. Chem.* **1985**, *26*(2), 74-76.

3. Theodorou, D.N.; Ludovice, P.J.; Suter, U.W. “Detailed Modeling of Structure and Deformation of Glassy Polymers”, in *Scattering, Deformation and Fracture in Polymers*; Crist, B.; Russell, T.P.; Wignall, G.D., Eds; Mat. Res. Soc. Symp. Proc. Vol.79; Materials Research Society: Pittsburgh, Pennsylvania, 1987; p 387-396.

4. Mansfield, K.F.; Theodorou, D.N. “Molecular Simulation of Glassy Polymer Surfaces” *Polym.Prepr., Am.Chem.Soc., Div.Polym.Chem.* **1988**, *29*(2), 402-403.

5. Theodorou, D.N. “Molecular Thermodynamics of Polymer Melts at Interfaces”, LBL Report No 26018, September 1988.

6. Mansfield, K.F.; Theodorou, D.N. "Molecular Modeling of Polymers at Interfaces" *Polym.Prepr., Am.Chem.Soc., Div.Polym.Chem.* **1989**, *30*(2), 76-77.

7. Mansfield, K.F.; Theodorou, D.N. “Molecular Dynamics of a Glassy Polymer Film” *Polym.Prepr., Am.Chem.Soc., Div.Polym.Chem.* **1992**, *33*(1), 691-692.

8. Dodd, L.R.; Theodorou, D.N. “Thermodynamic Properties of Alkanes and Polyethylene: Continuum Mean Field Theory and Monte Carlo Simulation” *Polym.Prepr., Am.Chem.Soc., Div.Polym.Chem.* **1992**, *33*(1), 645-646.

9. Boone, T.D.; Theodorou, D.N. “Monte Carlo Simulation of Bulk Glassy Polymers and Penetrant Sorption” *Polym.Prepr., Am.Chem.Soc., Div.Polym.Chem.* **1992**, *33*(1), 513-514.

10. Greenfield, M.L.; Theodorou, D.N. “Geometric Analysis of Diffusion Paths in Glassy Polymers” *Polym.Prepr., Am.Chem.Soc., Div.Polym.Chem.* **1992**, *33*(1), 689-690.

11. Bell, A.T.; Theodorou, D.N. “Applications of Molecular Dynamics and Transition State Theory to the Simulation of Diffusion in Zeolites”, in *Computer-Aided Innovation of New Materials II*; Doyama, M.; Kihara, J.; Tanaka, M.; Yamamoto, R., Eds.; Elsevier: Amsterdam, 1993; pp 991-996.

12. Snurr, R.Q.; Bell, A.T.; Theodorou, D.N. “Molecular Simulations of Low Occupancy Adsorption of Aromatics in Silicalite”, in *Proceedings of the 9th International Zeolite Conference, Montreal 1992*; von Ballmoos, R; Higgins, J.G.; Treacy, M.M.J., Eds.; Butterworth-Heinemann: Stoneham, 1993; pp 71-78.

13. Theodorou, D.N. “Molecular Modeling of the Interfacial Behavior of Amorphous Polymers: A Method for the Simulation of Fracture of Polymer/Polymer Interfaces”, in *ANTEC 93 Conference Proceedings, New Orleans, May 9-13, 1993*; Society of Plastics Engineers, 1993;

Vol. III, pp 3094-3096.

14. Pant, P.V.K.; Theodorou, D.N. "A Strategy for Atomistic Monte Carlo Simulation of Polydisperse Polymer Systems" *Polym.Prepr., Am.Chem.Soc., Div.Polym.Chem.* **1994**, *35*(1), 165-166.

15. Maginn, E.J.; Bell, A.T.; Theodorou, D.N. "Low-Occupancy Sorption Thermodynamics of Long Alkanes in Silicalite Via Molecular Simulation", in *Zeolites and Related Microporous Materials: State of the Art 1994*; Weitkamp, J.; Karge, H.G.; Pfeifer, H.; Hölderich, W., Eds.; Studies in Surface Science and Catalysis, vol. 84; Elsevier Science B.V.: Amsterdam, 1994; pp 2099-2105.

16. Greenfield, M.L.; Theodorou, D.N. "Description of Small Penetrant Jump Motions in a Polymer Glass Using Transition-State Theory", *Polymeric Materials: Science and Engineering* **1994**, *71*, 407-408.

17. Greenfield, M.L.; Theodorou, D.N. "Distribution of Jump Rate Constants Underlying Methane Diffusion in Glassy Atactic Polypropylene as Calculated With Transition-State Theory" *Polym.Prepr., Am.Chem.Soc., Div.Polym.Chem.* **1995**, *36*, 687-688.

18. Maginn, E.J.; Snurr, R.Q.; Bell, A.T.; Theodorou, D.N. ''Simulation of Hydrocarbon Diffusion in Zeolites'', in Progress in Zeolite and Microporous Materials; Chon, H.; Ihm, S.-K.; Uh, Y.S., Eds.; Studies in Surface Science and Catalysis, vol. 105C; Elsevier Science B.V.: Amsterdam, 1997; pp 1851-1858.

19. Gaub, M.; Fritzsche, S.; Haberlandt, R.; Theodorou, D.N. ''Transport and Self-Diffusion Coefficients in Zeolites: an MD Study'' *Proceedings of the 12th International Zeolite Conference*, Baltimore, MD 1998. M.M. Treacy, B.K. Marcus, M.E. Bisher, J.B. Higgins, Eds. Materials Research Society: Warrendale, 1999; pp 371-378.

20. Gergidis, L.N.; Theodorou, D.N.; Jobic, H. ''Dynamics of Alkane Mixtures in Silicalite Pores'' Proceedings of International workshop on Dynamics in Confinement, Grenoble, France, Jan 26-29, 2000. B. Frick, R. Zorn, H. Büttner, Eds. *J. Phys. IV France* **2000**, 10, Pr7 143-146.

21. Theodorou, D.N. ''Mobility of young researchers across Europe: Experiences from Participation in the TMR program'' Proceedings of the European Commission conference 'Investing in Europe's Human Research Potential' (4-7 October 2000, Crete, Greece), EU publication, Research Directorate - General, pp 48-52.

22. Theodorou, D.N. "Modeling Structure and Adhesion at Polymer/Polymer Interfaces", Proceedings of the International Symposium on Chain Molecules at Interfaces: Self-consistent Field Theory and Experiment, Wageningen, The Netherlands, August 2002, pp 52-54.

23. Peristeras, L.D.; Economou, I.G.; Theodorou, D.N. "Elementary Moves in Monte Carlo Simulation of Linear and Branched Polyolefins", poster presentation, proceedings of the 19th European Seminar on Applied Thermodynamics, Santorini, Greece, Sept. 2002, pp 169-172.

24. Raptis, V.E.; Melissas, V.E.; Economou, I.E.; Theodorou, D.N.; Sanopoulou, M.; Petrou, J.;

Petropoulos, J.H.; Finkelshtein, E.Sh.; Alentiev, A.; Yampolskii, Y.P. “Development of Novel Polymeric Membranes for Natural Gas Hydrocarbon Separation Through Experimental Measurements, Quantum Mechanics, Molecular Simulation and Macroscopic Modeling”, poster presentation, proceedings of the 19th European Seminar on Applied Thermodynamics, Santorini, Greece, September 2002, pp 173-177.

25. Jobic, H.; Makrodimitris, K.; Papadopoulos, G.K.; Schober, H.; Theodorou, D.N. “Diffusivities of CO_2 and N_2 in silicalite, comparison between quasielastic neutron scattering and molecular simulations’’, in *Recent Advances in the Science and Technology of Zeolites and Related Materials*, vol. 154(A-C); van Steen, E.; Callanan, L.H.; Claeys, M., Eds.; Studies in Surface Science and Catalysis, vol. 154(A-C); Elsevier: Amsterdam, 2004; pp 2056-2061

26. Logotheti, E.G.; Theodorou, D.N. “Computational Prediction of Polypropylene Melt Properties”, Proceedings of the 5th Panhellenic Scientific Conference in Chemical Engineering; Tziolas Editions: Thessaloniki, 2005; pp 153-156.

27. Tzoumanekas, Ch., Theodorou, D.N. “Topological Analysis of Entanglements in Polymer Melts”, Proceedings of the 5th Panhellenic Scientific Conference in Chemical Engineering; Tziolas Editions: Thessaloniki, 2005; pp 277-280.

28. 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”, Proceedings of the 5th Panhellenic Scientific Conference in Chemical Engineering; Tziolas Editions: Thessaloniki, 2005; pp 269-272.

29. Theodorou, D.N. “Hierarchical Simulations of Polymeric Materials”, *Abstr. Pap. Chem. Soc.* 230: 191 – PMSE, 2005.

30. Vergadou, N.; Theodorou, D.N. “Molecular Simulation for the Prediction of the Permeability of Glassy Polymers by Gases”, Proceedings of the 6th Panhellenic Scientific Conference in Chemical Engineering, NTU Athens, 2007; pp 149-152.

31. Tsalikis, D.; Peristeras, L.; Boulougouris, G.; Theodorou, D.N. “Computational Study of the Dynamical Properties of Glassy Polymers Using the Inherent Structure Picture”, Proceedings of the 6th Panhellenic Scientific Conference in Chemical Engineering, NTU Athens, 2007; pp 153-156.

32. Papadopoulos, G.K.; Theodorou, D.N. “Mesoscopic Simulations of the Diffusivity of Ethane in Beds of NaX Zeolite Crystals: Comparison with Pulsed Field Gradient NMR Measurements”, Proceedings of the 6th Panhellenic Scientific Conference in Chemical Engineering, NTU Athens, 2007; pp 285-287.

33. Tsalikis, D.; Peristeras, L.; Boulougouris, G.; Theodorou, D. “Parallel Programming Strategies for the Computation of Saddle Points in Multidimensional Potential Energy Surfaces”, Proceedings of the 6th Panhellenic Scientific Conference in Chemical Engineering, NTU Athens, 2007; pp 1305-1308.

34. Greenfield, M.L.; Theodorou, D.N. “Structure, Rate, and Mechanism of Methane Diffusion in Glassy Atactic Polypropylene”, *Polymeric Materials: Science and Engineering* **1997**, *76*,

429-430.

35. Vergadou, N.; Theodorou, D.N. “Microscopic Diffusion Mechanism of CO_2 in a Glassy Amorphous Polymer Matrix”, *diffusion-fundamentals.org* **2009**, *11*, 11.

36. Pantatosaki, E.; Papadopoulos, G.K.; Theodorou, DN. “Simulation Studies of CH_4, CO_2, H_2, and D_2 in FAU and MWW Framework Type Zeolites”, *diffusion-fundamentals.org* **2009**, *11*, 35.

37. 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” *diffusion-fundamentals.org* **2009**, *11*, 37.

38. Tsalikis, D.; Lempesis, N.; Boulougouris, G.C.; Theodorou, D.N. “Energy Lanscape-Based Study of Atomic Displacements in Glass Forming Materials” *diffusion-fundamentals.org* **2009**, *11*, 65.

39. Pantatosaki, E.; Papadopoulos, G.K.; Jobic, H.; Theodorou, D.N. “A Combined Simulation and Quasielastic Neutron Scattering Study of the Low-Temperature Dynamics of Hydrogen and Deuterium Confined in NaX Zeolite”, *diffusion-fundamentals.org* **2009**, *11*, 96.

40. Pazzona, F.G.; Sant, M.; Pantatosaki, E.; Papadopoulos, G.K.; Theodorou, D.N. “Analysis of Argon Diffusion in Zeolite Imidazolate Framework-8: Preliminary Calculations”, *diffusion-fundamentals.org* **2009**, *11*, 97.

41. Kolokathis, P.D.; Theodorou, D.N. “Computing diffusivities in spatially periodic media from the rate constants of elementary jumps between sorption sites: Master Equation Solution by Recursive Reduction of Dimensionality”, *AIChE Annual Meeting Conference Proceedings* **2012**, paper 278a.

42. Vogiatzis, G.G; Theodorou, D.N. “Chain conformations in polymer nanocomposites: A Field Theory-inspired Monte Carlo simulation approach”, *AIChE Annual Meeting Conference Proceedings* **2012**, paper 709a.

43. Moorthi, K.; Kamio, K.; Ramos, J.; Theodorou, D.N. “Stucture and entanglements in short chain branched polyolefin melts”, *AIP Conference Proceedings* **2013**, *1518*, 455-458.

44. Anogiannakis, S.D.; Tzoumanekas, C.; Georgilas, V.; Theodorou, D.N. “Molecular Modelling of Deformation and Fracture in Polymer Networks”, Proceedings of the 16th International Conference on Deformation, Yield, and Fracture of Polymers (DYFP2015), Rolduc, Kerkrade, The Netherlands, March/April 2015.

45. Ziogos, O.G.; Theodorou, D.N. “Structural and dynamical properties of nanographene molecular wires: A molecular dynamics study”, *IEEE 15th International Conference on Nanotechnology (IEEE-NANO)* **2015**, 817-820.

46. Koutsoumaris, C.C.; Vogiatzis, G.G.; Theodorou, D.N.; Tsamasphyros, G.J. “Application of bi-Helmholtz nonlocal elasticity and molecular simulations to the dynamical response of

carbon nanotubes", *International Conference of Computational Methods in Sciences and Engineering 2015 (ICCMSE 2015), AIP Conf. Proc.* **2015**, *1702*, 190011.

47. Megariotis, G.; Ziogos, O.G.; Theodorou, D.N. "Multiscale simulations of hexa-peri-hexabenzocoronene and hexa-n-dodecyl-hexa-peri-hexabenzocoronene" *International Conference of Computational Methods in Sciences and Engineering 2015 (ICCMSE 2015), AIP Conf. Proc.* **2015**, *1702*, 190010.

48. Megariotis, G.; Vogiatzis, G.G.; Schneider, L.; Müller, M.; Theodorou, D.N. "Mesoscopic simulations of crosslinked polymer networks" *J. Phys.: Conf. Ser.* **2016**, *738*, 012063.

49. Kritikos, G.; Sgouros, A.; Vogiatzis, G.G.; Theodorou, D.N. "Molecular dynamics study of polyethylene under extreme confinement" *J. Phys.: Conf. Ser.* **2016**, *738*, 012012.

50. Mathioudakis, I.; Vogiatzis, G.G.; Tzoumanekas, C.; Theodorou. D.N. "Molecular modeling and simulation of atactic polystyrene/amorphous silica nanocomposites" *J. Phys.: Conf. Ser.* **2016**, *738*, 012021.

51. Ziogos, G.; Megariotis, G.; Theodorou, D.N. "Atomistic and coarse-grained simulations of hexabenzocoronene crystals" *J. Phys.: Conf. Ser.* **2016**, *738*, 012019.

52. Romanos, N.; Megariotis, G.; Theodorou, D.N. "Molecular dynamics simulations of polyethylene bilayers" *J. Phys.: Conf. Ser.* **2021**, *1730*, 012039.

53. Evangelou, N.; Megariotis, G.; Sgouros, A.P.; Vogiatzis, G.G.; Romanos, N.A. "Coarse-grained simulations of bidisperse polymer melts" *AIP Conference Proceedings* **2021**, *2343*, 130008.

54. Philippas, A.P.; Sgouros, A.P.; Megariotis, G.; Theodorou, D.N. "Mesoscopic simulations of star polyethylene melts at equilibrium and under steady flow" *AIP Conference Proceedings* **2021**, *2343*, 130003.

55. Revelas, C.J.; Sgouros, A.P.; Lakkas, A.T.; Theodorou, D.N. "A three-dimensional finite element methodology for addressing heterogeneous polymer systems with simulations based on self-consistent field theory" *AIP Conference Proceedings* **2021**, *2343*, 130002.

56. Megariotis, G.; Romanos, N.A.; Theodorou, D.N. "Molecular simulations of dopamine in a lipid bilayer" *AIP Conference Proceedings* **2021**, *2343*, 130007.

57. Venetsanos, F.; Anogiannakis, S.D.; Theodorou, D.N. "Thermodynamic analysis of oligomeric blends by applying the Kirkwood-Buff theory of solutions" *J. Phys: Conf. Ser.* **2021**, *2090*, 012079.

58. Nasikas, D.; Ricci, E.; Giannakopoulos, G.; Karkaletsis, V.; Theodorou, D.N.; Vergadou, N. "Investigation of machine learning-based coarse-grained schemes for organic molecules" SETN 2022, September 07-09, Corfu, Greece, Association for Computing Machinery 2022, https://doi.org/10.1145/3549737.3549792.

59. Ricci, E.; Giannakopoulos, G.; Karkaletsis, V.; Theodorou, D.N.; Vergadou, N. “Developing machine-learned potentials for coarse-grained molecular simulations: challenges an pitfalls” SETN 2022, September 07-09, Corfu, Greece, Association for Computing Machinery 2022, https://doi.org/10.1145/3549737.35497923.

BIBLIOMETRIC DATA (August 2022)

ORCID https://orcid.org/0000-0002-4763-9739

Scopus https://www.scopus.com/authid/detail.uri?authorId=7005515056
249 documents, 13672 citations, h-index = 61
11340 citations, h-index = 54 if self-citations of all authors are excluded

Google Scholar https://scholar.google.gr/citations?user=leOswz4AAAAJ&hl=el
18841 citations, h-index = 71

Presentations 162 invited presentations in international scientific meetings, 95 invited talks at universities and national research laboratories, 31 invited talks at industrial research centers, 157 contributed presentations in scientific meetings.

FORMER GROUP MEMBERS AND THEIR CURRENT EMPLOYMENT

Vassilis Dendroulakis	Dipl.Th. NTUA, 2004	Process Engineer (MSAT), Moderna, Boston, MA, USA
Despina Tzoulaki	Dipl.Th. NTUA, 2005	Manager, Grant Thornton Greece, Athens, GR
Antonia Vyrkou	Dipl.Th. NTUA, 2005	Research Assistant in Industrial Symbiosis, Huddersfield University, UK
Stefanos Anogiannakis	Dipl.Th. NTUA, 2006	Post-doc, NTU Athens, GR
Nikolaos Lempesis	Dipl.Th. NTUA, 2007	Research Associate, EPFL, Lausanne, CH
Chrysanthos Constantinou	Dipl.Th. NTUA, 2008	M.S. Rutgers University, US, 2011
Manolis Haldoupis	Dipl.Th. NTUA, 2008	Data Management Specialist, BASF, Ludwigshafen, DE
Manolis Vasileiadis	Dipl.Th. NTUA, 2009	ERP/SCM Consultant, Oracle, Athens, GR
Eirini Siougkrou	Dipl.Th. NTUA, 2009	Senior Applications Consultant, Oracle, Athens, GR
Maria Pikoula	Dipl.Th. NTUA, 2009	Clinical Data Scientist, UCL, UK
Polydefkis Diamantis	Dipl.Th. NTUA, 2009	Bioinformatician, Hengrui Europe Biosciences Ltd., Zürich, CH
Georgios Vogiatzis	Dipl.Th. NTUA, 2010	Post-doc, NTU Athens, GR and Dutch Polymer Institute, Eindhoven, NL
Panagiotis Kolokathis	Dipl.Th. NTUA, 2010	Post-doc, NTU Athens, GR
Stylianos Karozis	Dipl.Th. NTUA, 2010	Project Manager/Collaborating Researcher, NCSR “Demokritos”, Athens, GR
Christina-Anna Gatsiou	Dipl.Th. NTUA, 2011	SNF Post-doc, NCSR “Demokritos”, GR
Phaedon Brotzakis	Dipl.Th. NTUA, 2012	FEBS Post-doctoral Individual Fellow, U. Cambridge, UK
Nick Stefanopoulos	Dipl.Th. NTUA, 2012	Senior Process Engineer, McCormick & Co., Peterborough, England, UK
Ioannis Petsagkourakis	Dipl.Th. NTUA, 2013	Researcher, RISE Institutes, Norrköping, SE
Andreas Gavrielides	Dipl.Th. NTUA, 2014	R&D Project Manager, eBOS, Nicosia, CY

Spyros Kournopoulos	Dipl.Th. NTUA, 2014	Numerics Software Developer, Siemens Digital Industries Software, London, UK
Ariadni Boziki	Dipl.Th. NTUA, 2014	Post-doctoral Researcher, University of Luxembourg, LU
Anastasia Nikolakopoulou	Dipl.Th. NTUA, 2015	Scientist, Process Operation and Modeling, Sanofi, Waltham, MA, US
Stefanos Konstantinopoulos	Dipl.Th. NTUA, 2015	Ph.D. Imperial College London, UK, 2020
Konstantinos Manikas	Dipl.Th. NTUA, 2015	Design Engineer, ASML, Veldhoven, NL
Virginia Abdol Hadi	Dipl.Th. NTUA, 2017	
Myrto Perdikari	Dipl.Th. NTUA, 2017	Scientist, Dewpoint Therapeutics, Boston, MA, USA
Michael Frangou	Dipl.Th. NTUA, 2017	Petrochemical Analyst, ICIS, London, UK
Konstantinos Zinelis	Dipl.Th. NTUA, 2017	Ph.D. student, Imperial College London, UK
Katerina Galata	Dipl.Th. NTUA, 2018	Ph.D. candidate, Polymer Physics, ETH Zürich, CH
Nikolas Evangelou	Dipl.Th. NTUA, 2018	Ph.D. student, Johns Hopkins Univ., USA
Vasilis Papasimakopoulos	Dipl.Th. NTUA, 2018	M.S. University of Chicago, USA, 2021
Matrona Panou	Dipl.Th. NTUA, 2018	Ph.D. student, NCSR “Demokritos” & NTUA
Vangelis Konialidis	Dipl.Th. NTUA, 2018	Chemical Analyst, Bureau Veritas Group, Athens, GR
Fotis Venetsanos	Dipl.Th. NTUA, 2018	Ph.D. student, NTU Athens, GR
Evgenia Kountoupi	Dipl.Th. NTUA, 2019	Ph.D. student, ETH Zürich, CH
Evangelos Tsochantaris	Dipl.Th. NTUA, 2019	Ph.D. student, DTU, DK
Alexandros Philippas	Dipl.Th. NTUA, 2019	Ph.D. student, Georgia Inst. of Technol., USA
Nikolaos Sigalas	Dipl.Th. NTUA, 2019	Ph.D. student, Univ. Eindhoven, NL
Christina Zois	Dipl.Th. NTUA, 2019	
Tzortzis Koulaxizis	Dipl.Th. NTUA, 2020	Ph.D. student, Univ. of Illinois at Urbana-Champaign, USA

Konstantina Karanasiou	Dipl. Th. NTUA, 2020	Process Engineer, Siemens Gamesa, Aalborg, DK
Evangelos Patounas	Dipl. Th. NTUA, 2020	Manufacturing Quality Technician, Philip Morris International
Leonidas Konstadopoulos	Dipl. Th. NTUA, 2021	
Ermioni Charalampopoulou	Dipl. Th. NTUA, 2021	Ph.D. student, USC, USA
Georgios Mikaelian	Dipl. Th. NTUA, 2021	Ph.D. student, NTUA
George Sakellion	Dipl. Th. NTUA, 2021	
Evangelos Drougkas	Dipl. Th. NTUA, 2021	Ph.D. student, DTU, Lyngby, DK
Dimosthenis Chalkiopoulos	Dipl. Th. NTUA, 2021	Guest Relations Agent, The Westin Resort, Costa Navarino, GR
Dimitrios Nasikas	Dipl. Th. NTUA, 2021	Ph.D. student, NCSR “Demokritos”, Athens, GR
Magda Karavangeli	Dipl. Th. NTUA, 2022	
Dimitris Tsagkalakis	Dipl. Th. NTUA, 2022	
Aikaterini Argyropoulou	Dipl. Th. NTUA, 2022	
Dimos Aslanis	Dipl. Th. NTUA, 2022	
Alexandros Timotheos Loukas	Dipl. Th. NTUA, 2022	

Sandra Maria Nelson	M.S. Berkeley, 1988	Process Engineer, Chevron Corporation, Richmond, CA, USA
Dimitra Angelopoulou	M.S. Patras, 2000	Intracom Hellas, Patras, GR
Georgia Tsolou	M.S. Patras, 2000	Instructor, University of Patras, GR
Georgia Schismenou	M.S. Patras, 2001	
Michael Apostolakis	M.S. Patras, 2001	
Christos Kyroudis	M.S. NTUA, 2009	Researcher, InSilico Oncology Group, ICCS, NTUA, GR

Harry Pitouras	M.S. NTUA, 2009	Ph.D., NTU Athens, GR
Aristides Troupis	M.S. NTUA, 2010	Ph.D., University of Patras, GR
Andreas Morphis	M.S. NTUA, 2012	
Georgios Vogiatzis	M.S. NTUA, 2012	Post-doc, NTU Athens, GR and Dutch Polymer Institute, Eindhoven, NL
Ioulia Tzouvadaki	M.S. NTUA, 2012	Marie Curie Research Fellow, University of Southampton, UK
Stelios Karozis	M.S. NTUA, 2013	Project Manager/Collaborating Researcher, NCSR “Demokritos”, Athens, GR
Chrisa Charitoglou	M.S. NTUA, 2013	Full Stack Developer, Public Soft PC, Athens, GR
Panagiotis-Nikolaos Tzounis	M.S. NTUA, 2014	Test analyst, ARHS Development Hellas, GR
Aris Sgouros	M.S. NTUA, 2015	Post-doc, NTU Athens, GR
Andreas Balafoutis	M.S. NTUA, 2016	Information Technology Engineer, ELANET, Athens, GR
Lefteris Koulierakis	M.S. NTUA, 2016	Data Scientist, ASML, Veldhoven, NL
Spyros Kournopoulos	M.S. NTUA, 2016	Numerics Software Developer, Siemens Digital Industries Software, London, UK
Dionysis Liveris	M.S. NTUA, 2017	Ph.D. student, NTU Athens, GR
George Kissas	M.S. NTUA, 2017	Ph.D. student, Univ. of Pennsylvania, US
Stefanos Konstantinopoulos	M.S. NTUA, 2017	Ph.D. student, Imperial College London, UK
Panos Petris	M.S. NTUA, 2018	Application Engineer, Siemens Digital Industries Software, The Hague, and Ph.D. candidate, Univ. of Leiden, NL
Dora Argyropoulou	M.S. NTUA, 2018	Researcher, Biomedical Research Foundation of the Academy of Athens, GR
Katerina Avramidou	M.S. NTUA, 2018	
Ioannis Haloulos	Res.stud. NTUA, 2016	Business Development Executive, Alfa Analytical Instruments, Athens, GR
Dimitris Paraskevas Gerakinis	M.S. NTUA, 2022	Ph.D. student, NCSR “Demokritos”, GR

Kevin Francis Mansfield	Ph.D. Berkeley, 1991	Global Director of Product Care, Evonik, Allentown, PA, US
Raymond Lawrence June	Ph.D. Berkeley, 1991	Global Technology Manager, SMPO & PO Derivatives, Shell Oil Co., Houston, TX, US
Randall Quentin Snurr	Ph.D. Berkeley, 1994	John Searle Professor and Chair of Chemical and Biological Engineering, Northwestern University, Evanston, IL, US
Travis David Boone	Ph.D. Berkeley, 1995	Biotechnology Development Consultant (SME), NASA Ames Res. Center, Mountain View, CA, US
Edward Joseph Maginn	Ph.D. Berkeley, 1995	Keough-Hesburgh Professor of Engineering and Associate Vice President for Research, Univ. of Notre Dame, Notre Dame, IN, US
Michael Lewis Greenfield	Ph.D. Berkeley, 1996	Associate Professor and Graduate Director of Chemical Engineering, University of Rhode Island, Providence, RI, US
Lawrence Benjamin Fischel	Ph.D. Berkeley, 1997	Lead, Modeling and Simulation, The Clorox Company, Pleasanton, CA, US
Theodora Spyriouni	Ph.D. Patras, 1998	Research Scientist, Scienomics SARL, Athens, GR
Stelios Antoniadis	Ph.D. Patras, 1999	ASF Production Manager, Polyeco SA, Athens, GR
Evangelia Zervopoulou	Ph.D. Patras, 2000	
Leonidas Gergidis	Ph.D. Patras, 2000	Associate Professor of Materials Science and Engineering, University of Ioannina, GR
Christina Samara	Ph.D. Patras, 2000	Manufacturing Manager, Eurofilm Mantzaris S.A., Corinth, GR
George Boulougouris	Ph.D. NTU Ath. 2001	Associate Professor, Molecular Biology and Genetics, U. of Thrace, Alexandroupolis, GR
Costas Chassapis	Ph.D. U. Athens 2001	Head of Software Engineering Department & Quality Management Director, Algosystems S.A., Athens
Vagelis Harmandaris	Ph.D. Patras, 2001	ERA Chair Professor, The Cyprus Institute, CY, and Professor of Mathematics and Applied Mathematics, University of Crete, GR

Manolis Doxastakis	Ph.D. Patras, 2001	Associate Professor of Chemical and Biomolecular Engineering, University of Tennessee, Knoxville, TN, USA
Konstantinos Makrodimitris	Ph.D. NTUA, 2002	Senior Advisor, US Dept. of Health and Human Services and FDA, MD, US
Nikos Karayiannis	Ph.D. Patras, 2002	Professor, Research Profile I3, Universidad Politécnica de Madrid, ES
Loukas Peristeras	Ph.D., U. Athens, 2004	Research Scientist, Institute of Nanoscience and Nanotechnology, NCSR "Demokritos", Athens, GR
Vasilios Raptis	Ph.D., U. Athens, 2004	Post-doctoral researcher, National Hellenic Research Foundation, Athens, GR
Nikos Kopsias	Ph.D., Patras, 2005	Business Development and Marketing Manager, Oxygen Broadband, GR
Georgia Evangelia Logotheti	Ph.D., NTUA, 2006	Associate Managing Consultant, Mastercard, Athens, GR
Niki Vergadou	Ph.D., U. Athens, 2006	Research Scientist, Institute of Nanoscience and Nanotechnology, NCSR "Demokritos", Athens, GR
Gregory Megariotis	Ph.D., NTUA, 2009	Post-doc, NTU Athens, GR
Dimitris Tsalikis	Ph.D., NTUA, 2009	Post-doctoral Research Fellow, U. of Patras, GR
Nikolaos Romanos	Ph.D., NTUA, 2009	Post-doc, NTU Athens, GR
Marco Sant	Ph.D., NTUA, 2010	Post-doc, Università di Sassari, IT
Stefanos Anogiannakis	Ph.D., NTUA, 2012	Post-doc, NTU Athens, GR
Antonia Vyrkou	Ph.D., NTUA, 2012	Research Assistant in Industrial Symbiosis, Huddersfield University, UK
Thanasis Morozinis	Ph.D., NTUA, 2013	R&D Scientist, Katradis Marine Ropes Industry SA, Piraeus, GR
Nikos Lempesis	Ph.D., NTUA, 2013	Research Associate, EPFL, Lausanne, CH
Georgios Vogiatzis	Ph.D., NTUA, 2015	Post-doc, NTU Athens, GR and Dutch Polymer Institute, Eindhoven, NL

Panagiotis Kolokathis	Ph.D., NTUA, 2016	Post-doc, NTU Athens, GR
Ioannis Mathioudakis	Ph.D., NTUA, 2016	Post-doc, CPERI/CERTH & University of Thessaloniki, GR
Orestis Georgios Ziogos	Ph.D. NTUA, 2018	Full Stack Software Engineer, Nokia, Athens, GR
Aris Sgouros	Ph.D. NTUA, 2019 Iacovos Giourounlian 1st Prize 2019	Post-doc, NTU Athens, GR
Spiros Kallivokas	Ph.D. NTUA, 2020	Post-doc, Hellenic Institute of Transport, CERTH, GR
Apostolos Lakkas	Ph.D. NTUA, 2021	Officer, Greek Armed Forces
Lawrence Robert Dodd	Post-doc, Berkeley	Director, Robydodd Family Charitable Foundation, Ridgefield, CT, US
Edith Marie Sevick	Post-doc, Berkeley	Professor, Research School of Chemistry, ANU, Canberra, AU
P.V. Krishna Pant	Post-doc, Berkeley	VP Bioinformatics, Deepcell, Inc., Mountain View, CA, US
Vlasis G. Mavrantzas	Post-doc, U. Patras	Professor, University of Patras, GR & Visiting Professor, ETH Zürich, CH
Magnus Ullner	Post-doc, U. Patras	Senior Lecturer, Theoretical Chemistry, University of Lund, SE
Rob H.C. Janssen	Post-doc, U. Patras	Principal Scientist, DSM, Geleen, NL
Jean-Marc Bomont	Post-doc, U. Patras	Chercheur associé HDR, Université de Lorraine, FR
Andreas Terzis	Post-doc, U. Patras	Professor of Physics, Univ. of Patras, GR
Oscar Ahumada	Post-doc, U. Patras	General Manager, Mecwins, Madrid, ES
Vassilios Melissas	Post-doc, “Demokritos”	Associate Professor of Chemistry, University of Ioannina, GR
Erwan Nicol	Post-doc, U. Patras	Maître de Conférences, Le Mans Univ., FR
Patricia Gestoso-Souto	Post-doc, U. Patras	Global Head, Scientific and Technical Customer Support, BIOVIA – Dassault Systèmes,

		Manchester, UK
George K. Papadopoulos	Post-doc, “Demokritos”	Associate Professor of Chemical Engineering, NTU Athens
Nikolas Zacharopoulos	Post-doc, “Demokritos”	Lecturer, Department of Product and Systems Design Engineering, University of the Aegean, Syros, GR
Christos Tzoumanekas	Post-doc, NTU Athens	Physics teacher, Greek high-school system
Collin D. Wick	Post-doc, NTU Athens	Century Tel Professor of Chemistry and Associate Dean of Graduate Studies, Louisiana Tech University, US
Kostas Daoulas	Post-doc, NTU Athens	Privatdozent, Group Leader, Max-Planck Institut für Polymerforschung, Mainz, DE
Jean-Marc Leyssale	Post-doc, NTU Athens	Research Scientist (HDR), Inst. des Sciences Moléculaires, CNRS Bordeaux, FR
Luigi Sanguigno	Post-doc, NTU Athens	Associate Researcher, University of Derby, UK
Kazunori Kamio	Visiting Researcher, NTU Athens	Researcher, Mitsui Chemicals, Sodegaura, JP
Francisco Javier Ramos-Díaz	Post-doc, NTU Athens	Researcher, CSIC, Madrid, Spain
Adrien Leygue	Post-doc, NTU Athens	Chargé de Recherche, CNRS Nantes, FR
Evangelos Voyiatzis	Post-doc, NTU Athens	Researcher, Novamechanics Ltd, Nicosia, CY
Maxime Delhorme	Post-doc, NTU Athens	Release train engineer, ASML, Veldhoven, NL
David Nieto-Simavilla	Post-doc, NTU Athens	Post-doc, Basque Center for Advanced Mathematics, University of Bilbao, ES
Maria Grazia de Angelis	Visiting Scientist, NTU Athens	Professor and Chair of Chem. Eng., University of Edinburgh, UK
Federico Pazzona	Visiting Post-doc, NTU Athens	Research Fellow, Universitá degli Studi di Sassari, IT
Lambèrt C.A. van Breemen	Visiting Scientist, NTU Athens	Assistant Professor, Eindhoven University of Technology, NL
Mark C. Thies	Marie Curie Internat.	Dow Chemical Professor of Chemical,

	Incoming Fellow	Egineering, Clemson University, SC, USA
Aaron Thornton	Visiting Scientist, NTUA	Senior Research Scientist, Materials Science, CSIRO, AU
Piotr Kowalczyk	Visiting Scientist, NTU Athens	Assistant Professor, Murdoch University, Perth, AU
Antonis Vakis	Visiting Scientist, NTU Athens	Professor, University of Groningen, NL
Eleonora Ricci	Visiting Student, NCSR “Demokritos”	Marie Curie Fellow, NCSR “Demokritos”
Miguel Herranz Feito	Visiting Student, NTU Athens	Ph.D. candidate, Universidad Politécnica de Madrid, ES

CURRENT MEMBERS OF RESEARCH GROUP

At NTU Athens: **Computational Materials Science & Engineering Group**

Dr. Stefanos Anogiannakis	Postdoctoral Researcher
Dr. Grigorios Megariotis	Postdoctoral Researcher
Dr. Nikolaos Romanos	Postdoctoral Researcher
Dr. Aris Sgouros	Postdoctoral Researcher
Dr. Georgios Vogiatzis	Postdoctoral Researcher
Vassilis Georgilas	Ph.D. student
Georgios Mikaelian	Ph.D. student
Matrona Panou	Ph.D. student
Constantinos Revelas	Ph.D. student
Fotis Venetsanos	Ph.D. student
Evangelia Gkatzogia	Diploma Thesis student
Chrysanthi Dib	Diploma Thesis student

Collaborating Members

Dr. Francisco Javier Ramos Díaz	Researcher,Inst.de Estructura de la Materia,CSIC,Madrid,ES
Dr. David Nieto-Simavilla	Post-doc, Univ. Bilbao, ES
Dr. Loukas Peristeras	Research Scientist, NCSR “Demokritos”, Athens
Dr. Niki Vergadou	Research Scientist, NCSR “Demokritos”, Athens

FUNDING OF CURRENT RESEARCH WORK

1. "Physical and Chemical Ageing of Amorphous Polymers by Molecular Simulation" (PEARL), Project 829t19 undertaken in collaboration with the Eindhoven University of Technology and funded by the Dutch Polymer Institute, Subtechnology Area PP2.1 Performance Polymers, 26 July 2019 – 4 July 2023, NTU Budget € 200 000.

2. "Multiscale Simulations of Polymers at Interfaces" (MuSiPolI), Research project funded by the Hellenic Foundation for Research and Innovation (H.F.R.I. or ΕΛ.ΙΔ.Ε.Κ.), 23 December 2019 – 22 December 2022, € 188 000.

3. "Molecular modelling of stretch-induced crystallization in polyethylene and polypropylene layers (PO-stretched), Project 831 undertaken in collaboration with the Eindhoven University of Technology and funded by the Dutch Polymer Institute, Subtechnology Area Polyolefins, 1 April 2020 – 31 March 2024, NTU Budget € 252 000.

4. "Coarse-grained Modeling Investigations of Polymer Adhesion for Solid State Batteries" Industrial Research Agreements with Solvay SA, Belgium, 21 September 2021 – 20 October 2023, € 120 000.

FUNDING OF PAST RESEARCH WORK IN GREECE

1. "Development of New Modified Polymers and Blends for Packaging Materials and Agricultural Applications", EPET II (Operational Program for Research and Technology) No 623, General Secretariat of Research and Technology (GSRT) of Greece, 1 January 1995 - 31 December 1997. Partners: ARGO SA (coordinator), CPERI-FORTH Thessaloniki, Plastika Kritis SA, IESL-FORTH Crete, University of Patras, ICE/HT-FORTH. DNT Budget: 69 270 ECU.

2. "Improvement of the Domestic Capacity for Recycling Used Lube Oils", EPET II No 550, Greek GSRT, 1 January 1995 - 31 December 1997. Partners: LPC Hellas (coordinator), MOTOR OIL Hellas, ICE/HT-FORTH, University of Patras, University of Crete. DNT Budget: 72 670 ECU.

3. ''Molecular-Based Approach to the Simulation of Polymer Fluid Flows in Processing Operations'' (MPFLOW), BRITE-EuRam BRPR-CT96-145, funded by the European Commission, 1 June 1996 - 31 May 1999. Partners: ETSII Madrid (ES), Dow Benelux (NL), Repsol Petroleo (ES), Shell Research B.V. (NL), ARGO SA, ICE/HT-FORTH (GR), Université Catholique de Louvain (BE), T.U. Delft (NL), ETH Zürich (CH). DNT Budget: 144 000 ECU.

4. "Calculation of the Density, Elasticity, and Viscosity of Polymer Melts from the Chemical Constitution of Chains", PENED (Program for Enhancing Research Potential) No 218-96Δ of the Greek GSRT, 1 July 1996 - 31 December 1998. Budget: 8 million GRD.

5. ''Modeling Polymer Adhesion'', Research Contract with DSM Research B.V., The Netherlands, 1 March 1998 - 1 March 2000. Budget: 46 000 ECU.

6. ''Design, Synthesis and Study of Novel Nonlinear Optical Materials'', TMR Network Contract

ERB- FMRX-CT96-0047, funded by the European Commission, 1 October 1996 - 30 September 2000. Partners: NHRF-IOPC (coordinator), ICE/HT-FORTH (GR), UMIST (UK), University of Lund (SE), Universität Hannover (DE), University of Bristol (UK), Trinity College Dublin (IE), Commissariat á l' Energie Atomique (FR). DNT Budget: € 198 000.

7. ''New Routes to Understanding Polymer Materials Using Experiments and Realistic Modeling'', TMR Network Contract ERB-FMRX-CT98-0176, funded by the European Commission, 1 March 1998 - 28 February 2002. Partners: UMIST (UK, cordinator), Université Libre de Bruxelles (BE), E.S.P.C.I. Paris (FR), Universidad Complutense de Madrid (ES), Heriot-Watt University (UK), ICE/HT-FORTH (GR), Max-Planck Institut für Polymerforschung (DE). DNT Budget: € 182 000.

8. ''Predictive Modeling of Polyester Barrier Properties'', Research Contract with BP-Amoco Chemical Company, U.S.A., 1 January 2000 – 31 December 2001. Budget: $60 000.

9. ''Experimental and theoretical study of polymer crystallization from stagnant and flowing melts''. PENED 99 Program (99EΔ 95), General Secretariat of Research and Technology of Greece (GSRT), 1 January 2000 – 30 June 2001. Partners: University of Patras (coordinator), IESL-FORTH, Crete, University of Athens. DNT budget: 19 million GRD.

10. ''Design of New, Environmentally Friendly Self-Adhesive Materials'' (DEFSAM), Competitive and Sustainable Growth program G5RD-CT-2000-00202, funded by the European Commission, 1 March 2000 -28 February 2003. Partners: E.S.P.C.I. Paris (FR, coordinator), Exxon Chemical Europe (BE), Beiersdorf AG (DE), Universidad Politécnica de Madrid (ES), ICE/HT-FORTH (GR). DNT Budget: € 429 915, of which € 214 958 were provided by the European Union (Full cost basis).

11. ''Molecular Modeling for the Competitive Molecular Design of Polymer Materials With Controlled Permeability Properties'' (PERMOD), Competitive and Sustainable Growth Program G5RD-CT-2000-00200, funded by the European Commission, 1 March 2000 – 31 October 2003. Partners: GKSS Forschungszentrum Geesthacht GmbH (DE, coordinator), NCSR ''Demokritos''(GR), CNR-IRMERC (IT), MSI Ltd. (UK), Air Liquide (FR). DNT Budget: € 336 830, of which € 168 415 were provided by the European Union (full cost basis).

12. ''Transport-optimised catalysts for crude oil conversion'' (TROCAT), Competitive and Sustainable Growth Program G5RD-CT-2001-00520, funded by the European Commission, 1 September 2001 – 31 August 2004. Partners: Universität Leipzig (DE, coordinator), Grace-Davison Europe GmbH (DE), Cepsa S.A. (ES), SINTEF (NO), WITEGA S.A. (DE), Universität Stuttgart (DE), Heyrovský Institute of Physical Chemistry, Academy of Sciences of the Czech Republic (CZ), Chemopetroleo S.A. (CZ), NCSR "Demokritos"(GR). DNT budget € 366 730, of which € 183 365 were provided by the European Union (full cost basis).

13. ''Polymer Molecular Modeling at Integrated Length/Time Scales" (PMILS), Competitive and Sustainable Growth Program G5RD-CT-2002-00720, funded by the European Commission, 1 May 2002 – 30 April 2005. Partners: ETSII Madrid (ES), CPERI-CERTH (EL), Borealis S/A (DK), Rhodia Recherches (FR), Imperial College of Science, Technology and Medicine (UK), Integrated Process Solutions ApS (DK), ICE/HT-FORTH (GR). DNT-V.G. Mavrantzas budget € 422 953, of which € 203 977 was provided by the European Union (full cost basis).

14. "Hierarchical Modeling of Deformation and Failure of Polymer Glasses", Dutch Polymer Institute Project No 430, 1 March 2003 – 28 February, 2006. Budget € 260 741, of which 75% was provided by DPI.

15. "Experimental and Theoretical Study of Polypropylene for Industrial Applications in Plastic Packaging Containers", PENED 2001 Program (01EΔ529), General Secretariat of Research and Technology of Greece (GSRT), 1 September 2002 – 31 August 2006. Partners: University of Ioannina (coordinator), University of Patras, NTU Athens, Plastika Thrakis S.A.. NTUA budget: € 40 122.

16. "Molecular Simulation Study of Ageing and Plasticity in Glassy Materials (SIMGLASS)", Human Resources and Mobility (Marie Curie) European Reintegration Grant 006674 funded by the European Commission, 1 February 2005 – 31 January 2006. Budget € 40 000.

17. "Computational Study of Physical Ageing and Plastic Deformation in Glassy Materials", PYTHAGORAS program funded by the Greek ministry of National Education and Religion, 1 March 2004 – 31 August 2006. Budget € 85 000.

18. "Intelligent Design of Nanoporous Sorbents (INDENS)", Human Resources and Mobility (Marie Curie) Research Training Network MRTN-CT-2004-005503 funded by the European Commission, 1 January 2005 – 31 December 2008. Partners: CNRS/MADIREL (FR, coordinator), University of Edinburgh (UK), J. Heyrovský Institute of Physical Chemistry (CZ), University of St, Andrews (UK), N.T.U. Athens (GR), Universität Leipzig (DE), SINTEF (NO), Institut Français du Pétrole (FR). NTUA budget € 273 765.

19. "Computer-aided molecular design of multifunctional materials with controlled permeability properties (MULTIMATDESIGN)", NMP Specific Targeted Research Project (STREP) NMP3-CT-2005-013644 funded by the European Commission, 1 March 2005 – 28 February 2008. Partners: GKSS (DE, coordinator), NCSR "Demokritos" (GR), L'Air Liquide S.A. (FR), Research Institute on Membrane Technology (IT), Accelrys Ltd (UK), Universiteit Leiden (NL), MatSim GmbH (CH), A.V. Topchiev Institute of Petrochemical Synthesis (RU), Politecnico di Milano (IT), Università di Bologna (IT), Mesodyn BV (NL). "Demokritos" budget € 173 117.

20. "Study of the effect of external pressure (during thermoplastic extrusion) on the morphology and dynamics of industrial polypropylene", PENED 2003 program (Program for Enhancing Research Potential) No 03EΔ856 of the Greek GSRT, 1 October, 2005 - 30 July 2009. Partners: University of Ioannina (coordinator), NTU Athens, University of Patras, University of Crete, Plastika Thrakis S.A. NTU Athens budget: € 62 518.

21. "Computational study of the effect of the rate of glass formation on the properties of glassy materials", Carathéodory program funded competitively by the Senate Committee of Basic Research of NTU Athens, 1 February 2007 – 31 January 2009. Budget € 15 000.

22. "Multiscale Modeling of Nanostructured Interfaces for Biological Sensors (MNIBS)", EU-NSF Specific Targeted Research Project (STREP) NMP3-CT-2005-016375 funded by the European Commission, 1 December 2005 – 31 August 2009. Partners: Universidad Politécnica de Madrid (ES, EU coordinator), NTU Athens (GR), ETH-Zürich (CH), University of Wisconsin (US coordinator), Northwestern University, Purdue University. NTUA budget € 283 800.

23. "Molecular Modeling of Cavitation in Polymer Melts and Rubbers" (MOCAVIPOL), Dutch Polymer Institute (Engineering Plastics/Rubber Technology) Project Number 650, 1 November 2007 – 31 October 2011. Budget € 331 899.

24. "Multi-Scale Modeling of Nano-Structured Polymeric Materials: From Chemistry to Materials Performance" (NANOMODEL), FP7-NMP-2007-SMALL-1 Collaborative Project No 211778, funded by the European Commission, 1 November 2008 – 31 October 2011. Partners: BASF SE (DE, coordinator), Technische Universität Darmstadt (DE), NTU Athens (GR), Friedrich-Alexander Universität Erlangen-Nürnberg (DE), Gritche Technologies SARL (FR), Forschungszentrum Jülich GmbH (DE), Culgi BV (NL), Centro Ricerche Plast-Optica SPA (IT), Université de Fribourg (FR), Universitá degli Studi di Trieste (IT), Robert Bosch GmbH (DE). NTUA budget € 294 000.

25. "Advanced Materials as CO_2 Removers: A Computational Study of CO_2 Sorption Thermodynamics and Kinetics" (AMCOS), FP7-NMP-2008-EU-India-2 Collaborative Project No 233502, funded by the European Commission, 1 January 2009 – 31 December 2012. Partners: NTU Athens (GR, EU coordinator), Universität Leipzig (DE), Universitá degli Studi di Sassari (IT), Institut de Recherches sur la Catalyse et l' Environnement de Lyon - CNRS (FR), National Environmental Engineering Research Institute, Nagpur (Indian Coordinator), Institute of Chemical Technology Mumbai, Indian Institute of Technology Madras, Indian Institute of Chemical Technology Hyderabad. NTUA Budget € 150 000.

26. "Predicting the Properties of Carbonaceous Pitches via Molecular Modeling" (AdvCarbonMatls), FP7-PEOPLE-IIF-2008 Marie Curie International Incoming Fellowship No 234999 to Professor Mark Thies, Clemson University, USA, 1 March 2009 – 31 August 2011. Budget € 100 110.

27. "Molecular Simulation of Glassy Materials", "Heraklitos II" programme in support of Ph.D. thesis of Nikolaos Lempesis, Contract No MI8346725, Ministry of Education, Lifelong Learning and Religious Affairs of Greece, 1 February 2011 – 31 August 2013. Budget € 38 750.

28. "Multiscale Computational Approach to the Design of Polymer Matrix Nanocomposites" (COMPNANOCOMP-DPI), Additional funding provided by the coordinator Dutch Polymer Institute to NTU Athens in connection with the EU COMPNANOCOMP project to support a post-doc in the NTU group, 1 October 2012 – 31 March 2013. Budget: € 27 741.

29. "Multiscale Computational Approach to the Design of Polymer Matrix Nanocomposites" (COMPNANOCOMP), FP7-NMP-2011-RUSSIA Collaborative Project No 295355, EU-Russia collaboration whose EU part is funded by the European Commission, 1 October 2011 – 30 September 2014. EU Partners: Stichting Dutch Polymer Institute (NL, coordinator), Rhodia S.A. (FR), NTU Athens (GR), Eindhoven University of Technology (NL), CNRS-LPMA (FR), General Electric (DE), European Centre for Nanostructured Polymers s.c.a.r.l. (IT), University of Ulm (DE). Russian partners: Lomonosov Moscow State University (coordinator), Institute of Macromolecular Compounds St. Petersburg, National Research Centre Kurchatov Institute, Software Company PhysChem Ltd. NTUA Budget: € 181 030.

30. "Mesoscopic Simulations of Viscoelastic Properties of Networks (MSVIS)", 1 January 2014 – 31 December 2014, Volkswagen Foundation via University of Göttingen, NTUA Budget: € 50 000.

31. “Molecular Simulation of Polymer Networks: Stress-Strain Relations, Cavitation, and Dynamics in Confinement” (NETSIM), Project 744 funded by the Dutch Polymer Institute, 1 July 2012 – 31 December 2017. NTUA Budget: € 647 479.

32. “Computational Lithography for Directed Self-Assembly: Materials, Models and Processes” (CoLiSA-MMP), FP7-ICT-2013-11 Collaborative Project No 619793, 1 November 2013 – 31 October 2016. EU Partners: Fraunhofer Gesellschaft zur Förderung der Angewandten Forschung E.V., DE (coordinator), Arkema France S.A. (FR), Agencia Estatal Consejo Superior de Investigaciones Cientificas (ES), Université Bordeaux I (FR), Comissariat à l' Énergie Atomique et aux Énergies Alternatives (FR), Georg-August Universität Göttingen Stiftung Öffentlichen Rechts (DE). NTUA Budget: € 320 837.

33. “Multiscale Simulations of Complex Polymer Systems” (MuSiComPS), Research project in collaboration with University of Patras, 1 March 2015 – 30 November 2020 (renewed annually), Limmat Stiftung, Zürich, CH (coordinator). NTUA Budget: € 377 387.

34. “Molecular Simulations of Surfactant Self-Assembly” (MSiSSA), “Coarse-Grained Simulations of Nonionic Surfactants” (CGSiNIS), and “Coarse-Grained Simulations of Surfactants” (CGSS), Industrial Research Agreements with Rhodia Operations, France, a part of the Solvay Company, 1 October 2017 – 17 October 2020 (renewed annually), € 215 000.

35. “Multiscale Modelling for the Design of Antifouling Copolymers”, Industrial Research Agreement with Rhodia Operations, a part of the Solvay Company, 1 June 2019 – 1 June 2021, € 130 000.

REFERENCES

Professor Pablo G. Debenedetti
Department of Chemical Engineering
Princeton University
A-217 Engineering Quadrangle
Princeton, NJ 08544
U.S.A.
pdebene@princeton.edu

Professor John M. Prausnitz
Department of Chemical Engineering
University of California, Berkeley
308 Gilman Hall
Berkeley, CA 94720
U.S.A.
prausnit@chem.berkeley.edu

Professor Alexis T. Bell
Department of Chemical Engineering
University of California, Berkeley
107 Gilman Hall
Berkeley, CA 94720
U.S.A.
bell@cchem.berkeley.edu

Professor Morton M. Denn
Levich Institute, Steinman Hall #1M
City College of New York
140th Street and Convent Ave
New York, NY 10031
U.S.A.
denn@levdec.engr.ccny.cuny.edu

Professor Arup K. Chakraborty
Department of Chemical Engineering
Massachusetts Institute of Technology
Room 66-544
77 Massachusetts Ave.
Cambridge, MA 02139, U.S.A.
arup@uclink.berkeley.edu

Professor em. Dr. Ulrich W. Suter
ETH Zürich
HCI H 503
Wolfgang-Pauli-Strasse 10
CH-8093 Zürich
SWITZERLAND
uwsuter@ethz.ch

Professor Jean-Paul Ryckaert
Laboratoire de Physique des Polymères
CP-223, Université Libre de Bruxelles
Boulevard du Triomphe
B-1050 Brussels, BELGIUM
jryckaer@ulb.ac.be

Professor Dr. Jörg Kärger
Fakultät für Physik und Geowissenschaften
Abteilung Grenzflächenphysik
Universität Leipzig
Linnéstraße 5
D-04103 Leipzig, GERMANY
kaerger@rz.uni-leipzig.de

Professor Masao Doi
Center of Soft Matter Physics and its Applications
New Main Building Room H 1114
Beihang University
37 Xueyuan Road, Haidian District
Beijing, CHINA 100191
masao.doi@buaa.edu.cn

Professor Keith E. Gubbins
Department of Chemical and Biomolecular Engineering
North Carolina State University
Raleigh, NC 27695-7905
U.S.A.
keg@ncsu.edu

Professor Costas Vayenas
Department of Chemical Engineering
University of Patras
GR-26500 Patras
GREECE
cat@chemeng.upatras.gr

Professor Andreas Boudouvis
Rector
National Technical University of Athens
Zografou Campus, 157 80 Athens
GREECE
boudouvi@chemeng.ntua.gr