

DOROS NICOLAS THEODOROU  
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 Department of Materials Science and Engineering  
 School of Chemical Engineering  
 National Technical University of Athens  
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**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**

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

Warren K. Lewis Lecturer, Department of Chemical Engineering, Massachusetts Institute of Technology, March 2023.

“Doros N. Theodorou Festschrift”, [Virtual Special Issue](#) of the *Journal of Physical Chemistry B* (vol. 127, Number 12, March 30, 2023) edited by Edward J. Maginn, Ioannis G. Economou, Randall Q. Snurr, and Arup K. Chakraborty on the occasion of 65<sup>th</sup> birthday.

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), 2020-2023.

Member, Scientific Steering Committee, PRACE (Partnership for Advanced Computing in Europe), 2020-2023.

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, Bodossaki 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 Vlas G. Mavrantzas, special issue of the journal *Polymers on Coarse-Grained Models for Polymers*, 2023.

[https://www.mdpi.com/journal/polymers/special\\_issues/Cor\\_Gra\\_Mod\\_Poly](https://www.mdpi.com/journal/polymers/special_issues/Cor_Gra_Mod_Poly)

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, 9<sup>th</sup> 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 2023, 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, 12<sup>th</sup> edition (PPEPPD 2010), Suzhou, China, and 10<sup>th</sup> 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, 11<sup>th</sup> 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, 19<sup>th</sup> 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 and 2023-.

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, 2006-2014.

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

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

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

Member of Steering Committee and Instructor, Interdepartmental 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 ETH Zürich (CH), 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 organizations: European Research Council (Advanced and Consolidator grants), National Science Foundation (USA), INTAS Program, European Commission Marie Skłodowska-Curie Postdoctoral Fellowships, 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<sub>6</sub> 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. "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. Kyrilidis, 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 2<sup>nd</sup> 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.
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**Scopus** <https://www.scopus.com/authid/detail.uri?authorId=7005515056>  
 267 documents, 15183 citations, h-index = 63  
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**Google Scholar** <https://scholar.google.gr/citations?user=leOswz4AAAAJ&hl=el>  
 21803 citations, h-index = 75

**Presentations** 166 invited presentations in international scientific meetings  
 102 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

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| Georgios Vogiatzis      | Ph.D., NTUA, 2015<br>Best Thesis Award in Computational Mechanics, GRACM         | Post-doc, NTU Athens, GR and Dutch Polymer Institute, Eindhoven, NL                                                      |
| Panagiotis Kolokathis   | Ph.D., NTUA, 2016                                                                | Computational Scientist, Novamechanics Ltd, Nicosia, CY                                                                  |
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| Orestis Georgios Ziogos | Ph.D. NTUA, 2018                                                                 | Full Stack Software Engineer, Nokia, Athens, GR                                                                          |
| Aris Sgouros            | Ph.D. NTUA, 2019<br>Iacovos Giourounlian 1st Prize 2019<br>D. Chorafa Prize 2019 | Assistant Researcher, Theoretical and Physical Chemistry Inst., National Hellenic Research Foundation (NHRF), Athens, GR |
| Spiros Kallivokas       | Ph.D. NTUA, 2020                                                                 | Post-doc, Cyprus Institute, Nicosia, CY                                                                                  |
| Apostolos Lakkas        | Ph.D. NTUA, 2021                                                                 | Officer, Greek Armed Forces                                                                                              |
| Constantinos J. Revelas | Ph.D. NTUA, 2023                                                                 | Full-time Software Engineer, Teracloud Hellas, Attica, GR                                                                |
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| Jean-Marc Bomont       | Post-doc, U. Patras    | Chercheur associé HDR, Université de Lorraine, FR                                                        |
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| Oscar Ahumada          | Post-doc, U. Patras    | General Manager, Mecwins, Madrid, ES                                                                     |
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| 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       |
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| Nikolas Zacharopoulos  | Post-doc, “Demokritos” | Lecturer, Department of Product and Systems Design Engineering, University of the Aegean, Syros, GR      |
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| Collin D. Wick         | Post-doc, NTU Athens   | Century Tel Professor of Chemistry and Associate Dean of Graduate Studies, Louisiana Tech University, US |
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|-----------------------------|---------------------------------------|------------------------------------------------------------------------------|
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| 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, Università 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. Incoming Fellow | Dow Chemical Professor of Chemical, Engineering, Clemson University, SC, USA |
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| Stan van Kraaij | Visiting Researcher,<br>NTU Athens<br>(practical training) | MS student, Physics, Technische Universiteit<br>Eindhoven, NL |

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| Dr. Aristotelis Sgouros       | Postdoctoral Researcher     |
| Dr. Georgios Vogiatzis        | Postdoctoral Researcher     |
| Dimitris-Paraskevas Gerakinis | Ph.D. student (HFRI Fellow) |
| Georgios Mikaelian            | Ph.D. student (HFRI Fellow) |
| Matrona Panou                 | Ph.D. student               |
| Fotis Venetsanos              | Ph.D. student (HFRI Fellow) |
| Andreas Kolitsis              | M.S. student                |
| Chrysanthi Ntib               | Diploma Thesis student      |
| Nikolaos Panagiotopoulos      | Diploma Thesis student      |
| Nikolaos Papamatthaiakis      | Diploma Thesis student      |
| Dimitris Tryfonas             | Diploma Thesis student      |
| Dimitris Chrysafogeorgos      | Diploma Thesis student      |

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| Dr. Niki Vergadou               | Principal Researcher, NCSR “Demokritos”, Athens                 |
| Dr. Spyros Kallivokas           | Post-doc, Cyprus Institute, Nicosia, CY                         |
| Dr. Constantinos Revelas        | Post-doc, NTU Athens                                            |
| Dimos Aslanis                   | M.S. student, NTU Athens.                                       |
| Evangelos Drougkas              | Ph.D. student, DTU, Lyngby, DK                                  |

## 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 – 31 August 2024, NTU Budget € 200 000.
2. “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.
3. “Development of a multi-model for the simulation of the structural and mechanical properties of silica-rubber composites”, Industrial Research Agreement with Solvay SA, Belgium, 1 November 2022 – 31 October 2024, providing the salary of post-doctoral associate Dr. Georgios Vogiatzis.
4. “Modeling reaction-induced phase separation for the production of thermoplastic-toughened thermosets”, Industrial Research Agreement with Solvay Specialty Polymers, USA, LLC/SyensQo SA, Belgium, 1 July 2023 – 31 December, 2024, € 110 000.

## 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 à 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, coordinator), 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 (99EA 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” (MOCVIPOL), 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), Università degli Studi di Trieste (IT), Robert Bosch GmbH (DE). NTUA budget € 294 000.
25. “Advanced Materials as CO<sub>2</sub> Removers: A Computational Study of CO<sub>2</sub> 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), Università 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 Lempeis, 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” (COMPANOCOMP-DPI), Additional funding provided by the coordinator Dutch Polymer Institute to NTU Athens in connection with the EU COMPANOCOMP 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” (COMPANOCOMP), 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 Científicas (ES), Université Bordeaux I (FR), Commissariat 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.
36. “Multiscale Simulations of Polymers at Interfaces” (MuSiPoll), Research project funded by the Hellenic Foundation for Research and Innovation (H.F.R.I. or E.A.I.A.E.K.), 23 December 2019 – 22 December 2022, € 188 000.
37. “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.



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